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The news magazine of the International Union of Pure and Applied Chemistry (IUPAC)

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Front cover: Istanbul: Aya Sofya (Hagia Sophia—the Church of the Holy Wisdom) built 532–537AD in the reign of the Emperor Justinian. Before it became a Mosque (after the Turkish conquest) it was the largest Christian Church, it is now a museum.

International Union of Pure and Applied Chemistry

Istanbul 1995

The 35th Biennial Congress of the International Union for Pure and Applied Chemistry, organised in 1995 by the Turkish Chemical Society, was held in Istanbul at the Swissotel.

The hosting city, Istanbul—previously known as Constantinople, is the only city in the world built on two continents. The city stands on the shores of the Bosphorus where the waters of the Black Sea mingle with the Sea of Marma. On its truly majestic site, Istanbul contains the relics and splendour of the three empires of which it has been the capital.

Byzantium was a Greek town, founded by the Megarian King Byzas, which had been in existence for nearly nine centuries when it was chosen, in 330, by the Roman Emperor Constantine as his new capital city in the East of the Roman Empire; for political and military reasons he had decided to break the Roman Empire definitively into two halves. Rome was the capital of the Western Empire and the refounded Byzantium was to be the capital of the Eastern Empire. Indeed, when the Empire in the west was over run by barbarian armies in the 5th century, and after Rome had been sacked by the Vandals, the Roman Empire continued in the East with Byzantium becoming 'New Rome' and maintaining Roman culture and civilization. However, the Roman Empire was by this time a Christian Empire, and the original Latin tongue of Constantine had been replaced by the Greek language. The city becoming the center of the Orthodox Faith.

This Byzantine Empire continued to flourish for the next nine centuries reaching its apogee in the 10th Century under the Emperor Basil *Bulgaroctonus* (II) when the population of the city protected by its massive 5th century walls, almost 15 km in length, was well in excess of one million, at a time when Paris and London were relatively insignificant villages. However, with the advent of the Crusades, the Byzantine Empire was weaken from strife with Western Europeans, the Western Church and the Islamic World. With foes pressing from all sides, the empire continued to shrink and eventually the city of Byzantium was all that remained of the Byzantine Empire. The city was finally captured by the Ottoman Sultan Mehmed *the Conqueror* (II) on 29 May 1453, who refounded Byzantium as a Muslim city.

This was, however, not the end of the success of the city as the Turkish conquerors created the Ottoman Empire which dominated the Middle-East and Eastern Europe until the beginning of the present century and established their capital in Constantinople. However, with the dismemberment of the Ottoman Empire after the First World War, Constantinpole, which had by know become Istanbul, remained one of the great cosmopolitan cities of the Mediterranean.

It is ironical in that the Turkish name for the city is perhaps a corruption of the medieval Greek words '*'s tin polin*', which may be translated as 'going to town'—a familiar expression for those who live near a large town or city. The Greeks insist that the name of the city be Contantinople, a word never used by their Byzantine ancestors, but used by their Arab enemies and by the Prophet himself in the form Konstantiniye. Others say that Istanbul is a corruption of the Turkish expression '*Islambol*'—where Muslims are plentiful. Whatever, the origin of its modern name, the city dominated the imaginations of medieval people, the Slavs referred to the city as Tsarigard—the Emperor's city; and the Norsemen called it Micklegarth—the place between earth and the abode of the gods.

The opening cer-

Prof. A. Riza Berkem, President of the 35th IUPAC Congress and President of the Turkish Chemical Society.

emony of the 35th IUPAC Congress was held on the Monday morning in the ATATÜRK KÜLTÜR MERKEZI. The Organizing Committee, represented by Profs A.R. Berkem and B. Baysal spoke in English and welcomed the delegates to Istanbul. The Mayor and Governor of Istanbul both spoke in Turkish and repeated the welcome of the Organizing Committee. Prof. A.E. Fischli, Vice-President of the Union, spoke on behalf of IUPAC and introduced the Union to the delegates. Prof. Fischli described IUPAC, its history, its goals and spoke of how it goes about achieving these important tasks; he spoke about IUPAC's funding and about the numerous important international collaborations within which IUPAC is involved. The final comments at this ceremony of welcome were from the President of the Turkish Republic, His Excellency Süleyman Demirel, who had sent a message of welcome which was read, in both Turkish and English, to the delegates.

The organising committee of the 35th IUPAC Congress put together a scientific programme which covered a wide variety of different fields of chemistry, a wide ranging survey of the present state of knowledge and future trends in six areas of chemistry.

The opening ceremony was followed by a short intermission, after which the scientific programme began.

Human needs through chemistry

- Environment;
- Food;
- Energy;
- Health;

The Food Chemistry section contained one invited lecture (from Europe), three oral presentations and 39 posters. In the section on Health Chemistry, there were two invited lectures (US and Canada), 14 oral presentations and 76 poster presentations. In Energy, there were three invited lectures (all from the US), 5 oral presentations and 16 poster presentations. In the Environmental Chemistry section, there were two invited lectures (both from Turkey), 14 oral presentations and 97 poster presentations.

One of the interesting posters in the section on Environmental chemistry came from the group of Prof Abraham Clearfield at Texas A&M University, Texas, USA, relating to the design of new ion exchange materials which could operate under adverse conditions—*Ion exchange materials for nuclear and environmental waste remediation*.

There is a continuing need for stable selective ion exchange materials for nuclear and industrial waste treatment. In the case of nuclear waste resulting from weapons production, ion exchange materials have to be stable to high energy particles and to very corrosive chemical environments, for example, 1–3 Molar NaOH

Dr Faruk Demiray, Member of the Organizing Committee of the 35th IUPAC Congress and Secretary General of the Turkish Chemical Society.

and/or 1–2 Molar HNO_3. In addition, the exchange materials must have high selectivity for the ions of interest, as the solutions will contain high levels of a variety of salts. Under these conditions, organic resins are not suitable and one must move to new inorganic materials.

The synthesis and structure of a variety of layered and tunnel structures was described. These included several new titanates and zirconates, phosphates, silicophosphates, titanosilicates and pharmacosiderites. The high selectivity of these exchange materials recommends them for use in industrial and nuclear environments.

Physical chemistry, dynamics and structure

- Fast chemical processes;
- Energy transfer;
- State-to-state chemistry;
- Multiphoton and multiple photon excitation;
- Mode-selective chemistry;
- Theoretical calculations of reaction surfaces;
- Chemical kinetics;
- Molecular thermodynamics;
- Computational chemistry;
- Laser and molecular beams;
- Corrosion and its prevention.

The Physical Chemistry section of the Congress contained six invited lectures, three from Europe, one from the Middle East and two from the US. In addition, there were 30 oral presentations and 183 poster presentations. Of this total number of presentations, over half came from chemists in the geographical region of Turkey and the Middle East, and another 31% came from Asia.

Of particular interest was the lecture by Prof. R.D. Levine (Fritz Haber Research Center for Molecular Dynamics, The Hebrew University, Jerusalem) who spoke on the current developments in molecular reaction dynamics—*Molecular reaction dynamics looks towards*

Ferries wait to carry passengers across the Bosporus.

the next century: understanding complex systems.

The speaker showed how reaction dynamics is making increasing contact with real chemical systems by examining: elaborate reaction mechanisms typical of organic chemistry, the study of chemical reactions where the medium plays an active part (as is often the case on surfaces and in solution) and the mimicking of systems of biochemistry.

Much of the early conceptual ideas in this field came from the study of isolated, simple chemical exchange reactions where one chemical bond is broken as another is formed. A central feature of such reactions is the high selectivity which can be achieved by the choice of initial conditions and the specificity of the products. For example, the specificity of the energy dispersal of exoergic reactions—those that can produce chemical lasers. Prof. Levine pointed out that such ideas can now be increasingly carried over to more complex systems.

Organic chemistry, synthesis, mechanisms and natural products

- Bio-organic chemistry;
- Organometallic chemistry;
- Physical organic chemistry, organic electrochemistry;
- Organic photochemistry;
- Biosynthesis;
- Identification of natural products;
- Natural products with potential pharmacological activities.

In Organic chemistry, there were eight invited lectures, three from Europe, two from the US, two from the Middle East and one from Asia. In addition, there were 71 oral presentations and 204 posters. Of this total number of presentations, over half came from chemists in the geographical region of Turkey and the Middle East, and another 28% came from Asia.

Polymer science and high technology materials

- New methods of polymerization;
- Structure and properties of macromolecules;
- Solution properties of macromolecules;
- Engineering polymers and high performance materials;
- Polymeric blends and networks;
- Liquid crystalline polymers;
- Novel polymers have biological significance.

In the Polymer and Materials Chemistry section of the Congress there were nine invited lectures, five from Europe, one from the US, one from the Middle East and two from Asia. In addition, there were 39 oral presentations and 181 posters. Of this total number of presentations, almost two thirds came from chemists in the geographical region of Turkey and the Middle East, and another 25% came from Asia.

Analytical chemistry and instrumentation

- Computer based analytical methods;
- Electroanalytical methods;
- Atomic spectrometry;
- Molecular spectroscopy;
- Analytical separations and chromatography;
- Analytical separations in clinical science, analytical automation;
- Optical, electrochemical, acoustic, biological, and other sensors;
- Chemometrics, enzymatic techniques, capillary electrophoresis;
- Surface analysis;
- Flow injection analysis.

In Analytical Chemistry, there were nine invited lectures, six from Europe, two from the Middle East and one from the US. In addition, there were 33 oral presentations and 129 poster presentations. Of this total

Sultanahmet Camii (Blue Mosque) Built in the reign of Sultan Ahmet I (1603–1618).

number of presentations, over half came from chemists in the geographical region of Turkey and the Middle East, and another 24% came from Asia.

Inorganic chemistry and solid state

- Intermetallic compounds;
- New advanced inorganic materials;
- Coordination chemistry, electrochemistry of coordination compounds;
- Bio-inorganic chemistry;
- Inorganic photochemistry and photoelectrochemistry;
- Organometallic and cluster chemistry;
- Rare earth chemistry;
- Optoelectronics, crystals, thin films;
- Condensed phase chemistry;
- Catalysts and related subjects;
- Superconductors, semiconductors, organic conductors, solid state ionic conductors.

In the Inorganic Chemistry section of the Congress, there were four invited lectures, one from Europe and three from Asia. In addition, there were 41 oral presentations and 153 posters. Of this total number of presentations, over half came from chemists in the geographical region of Turkey and the Middle East, and another 22% came from Asia.

Of particular interest was an invited talk by Rüdiger Kniep (Eduard-Zintl-Instute, TH-Darmstadt, Germany) on a new class of inorganic materials—*Ternary and Quaternary Metal Nitrides: A new challenge for solid state chemistry*.

Compared with the large number of well known oxometalates, the crystal structure and chemistry of nitridometallates is still in its infancy. Of particular interest is the role of the nitride ion, which has a high polarizability and may therefore cause specific properties in structure and bonding. The important step in the investigation of these materials was the use of elemental nitrogen as an oxidizing agent for intermetallic melts.

Also of interest was an invited talk by Norman N. Greenwood (The University of Leeds, Leeds, UK)—*Recent developments concerning the discovery of elements 101–110*.

Professor Greenwood spoke of the ten newest elements ($Z = 101–110$) and their subsequent troubled history. How the preparation of these elements required outstanding feats of intellectual and experimental virtuosity—only a few short lived atoms are produced in several weeks of experimenting. However, some of the discoveries have been widely accepted, but others have been hotly contested.

There were five Plenary Lectures, a summary of these excellent and informative talks are given below:

Jack G. Calvert (National Center for Atmospheric Chemistry, USA)

The Chemistry of the Atmosphere, Its Perturbations Through Human Activities

The chemistry of the atmosphere results from a complex series of chemical reactions that involve many atmospheric trace gases and which are initiated through sunlight absorption by ozone, formaldehyde and other molecules which are present in the atmosphere in minute amounts. Within the troposphere, this complex photochemistry forms ozone and many other reactive intermediates including acids and peroxides. In contrast, stratospheric chemistry leads to the destruction of natural stratospheric ozone—our protective shield against hard ultraviolet solar radiation. This lose arises when halocarbons, normally unreactive compounds in the troposphere, are released at the surface of the Earth and are ultimately transported to the stratosphere. Here sunlight dissociated the halocarbons into highly reactive species that start chain reactions which can destroy atmospheric ozone.

Of current interest is the design and operation of environmentally friendly supersonic aircraft for the 21st century. Such new aircraft will have the same problem posed by the Anglo-French *Concorde* in the early 1970s, namely, the effect of the planes' nitrogen radical emissions on the ozone layer through which the plane flies. In the stratosphere, nitric oxide and nitrogen dioxide take part in complex catalytic reaction cycles that were previously thought to be the dominant process for ozone destruction throughout most of the lower strato-

sphere. Consequently, the greater the number of aircraft travelling through the ozone layer the greater the destruction.

Recent measurements reveal however that in the lower stratosphere (16–20 km altitude) the effect of nitrogen oxides on ozone is far outweighed by the ozone destroying reactions of hydrogen containing radicals, hydroxyl (OH) and hydroperoxyl (HO_2) and the halogen containing radicals such as chlorine monoxide (ClO) and bromine monoxide (BrO). Small additions of nitrogen radicals at those altitudes actually decreases the loss of ozone because the nitrogen containing radicals react with the hydrogen and halogen containing radicals thereby short circuiting their destructive effect. However, the impact on total ozone concentrations is uncertain due to the complexity of circulation and mixing models in the stratosphere.

Central to these new insights into nitrogen radical chemistry in the lower stratosphere are simultaneous measurements of the concentrations of all of the families of radicals that are involved in ozone destruction.

In contrast to earlier models that predicted a much more important role for NO_x catalysis, the cycles:

$$NO + O_3 \rightarrow NO_2 + O_2$$

$$NO_2 + O \rightarrow NO + O_2$$

Net: $O_3 + O \rightarrow 2O_2$

and

$$NO + O_3 \rightarrow NO_2 + O_2$$

$$NO_2 + O_3 \rightarrow NO_3 + O_2$$

$$NO_3 + \text{light} \rightarrow NO + O_2$$

Net: $2O_3 \rightarrow 3O_2$

account for less than 20% of the total ozone loss.

As a result of the enormous quantity of halocarbons dumped into the atmosphere over the last few decades, nearly one-third of the photochemical loss of ozone is due to reactions involving ClO and BrO radicals. The most important processes are:

$$HO_2 + ZO \rightarrow HOZ + O_2$$

$$HOZ + \text{light} \rightarrow OH + Z$$

$$Z + O_3 \rightarrow ZO + O_2$$

$$OH + O_3 \rightarrow HO_2 + O_2$$

Net: $2O_3 \rightarrow 3O_2$

where Z = Cl accounts for about 30% of halogen controlled loss and Z = Br accounts for between 20 and 30%. The reaction set

$$BrO + ClO \rightarrow Br + Cl + O_2$$

$$Br + O_3 \rightarrow BrO + O_2$$

$$Cl + O_3 \rightarrow ClO + O_2$$

Net: $2O_3 \rightarrow 3O_2$

is responsible for 20–25% of the halogen controlled loss. Finally,

$$O + ClO \rightarrow Cl + O_2$$

$$Cl + O_3 \rightarrow ClO + O_2$$

Net: $O + O_3 \rightarrow 2O_2$

accounts for 5% of ozone loss by halogen chemistry at 15km altitude, increasing to 25% at 21 km altitude. The formation of $ClONO_2$ and $BrONO_2$ leads to ozone loss through photolysis of NO_3 followed by the above reaction. These processes account for 10–15% of the halogen controlled loss rates.

Richard R. Ernst (ETH, Zurich, Switzerland)
Exploring the Structure and Dynamics of Molecules Through Nuclear Magnetic Resonance

Prof. Ernst began his lecture pointing out that 1995 was an anniversary year for scientists interested in structural studies. It was in 1945 that the first Nuclear Magnetic Resonance (NMR) spectra were obtained; a technique which is now one of the most versatile means of obtaining detailed molecular information on dynamics and structure. However, we are in addition to this anniversary celebrating the centenary of the discovery of x-rays; the other technique which gives detailed structural information. Prof. Ernst used his talk to demonstrate the versatility of NMR for the study of the dynamics and structure of a number of small polypeptide (ten amino acids), and how the observed molecular dynamics change with experimental conditions. For example, he demonstrated how the conformation of a cyclic decapeptide (antanamide), which from statistical arguments could assume any one of thousands of possible conformations, could be locked into one particular structure by a single water molecule which rapidly exchanged between polar side grouped on the polypeptide. NMR being the ideal tool for probing such dynamics.

Similarly, whereas X-rays can show you where the side chained dangling from a polypeptide attach themselves to another cellular component, X-rays cannot tell you the timescale on which this interaction is taking place. One can obtain a 'snap shot' of the overall structure, but with X-rays one cannot look into the nature of the interactions.

The speaker pointed out that the first NMR spectra gave little information of use to chemists, indeed, the early NMR scientists were all physicists or mathematicians. However, with the development of multi-dimensional Fourier transform NMR over the last 30 years, chemists can now obtain detailed information on intermolecular and intramolecular structure and dynamics. Indeed, NMR has recently developed into a leading diagnostic tool for the medical sciences, and is now an expensive item on one's hospital bill.

In some ways the techniques of NMR and X-rays are complimentary, however, they are also two competing tools for investigating similar properties. NMR is traditionally used to probe large molecules in solution where, for example, biological molecules are active - one can study the proteins in action. X-rays, however, give poorly resolved structural information on liquids, but give structures of the molecules in the solid state - X-rays cannot study protein function. Both NMR and X-rays can be used to determine crystal structure, X-rays have been used for this type of study in small molecules since the First World War. However, with large molecules of biological importance, for example, proteins, NMR can be used to determine structures of molecules ranging in size up to the kilodalton mass range—the smaller end of the protein market. X-rays, however, can be used to investigate the structure of the very largest proteins—megadalton mass range.

Rudolph A. Marcus (California Institute of Technology, USA)
Electron Transfer in Chemistry and Biology: Theory and Experiment

Prof. Marcus demonstrated how the field of electron transfer reactions has grown considerably from the late 1940s and early 1950s. During that period, the rates of many isotope exchange electron transfer reactions were determined using radioactive isotopes which had recently become available. Such reactions represented the simplest case of all chemical reactions, and electron transfer reactions in particular. Since this time when electron transfer reactions were considered a 'dusty corner' of a very specialized field of solution chemistry, the electron transfer field has grown to include many areas: inorganic reactions in solution; organic reactions; reactions at metal/liquid, semiconductor/liquid and liquid/liquid interfaces, and at modified electrodes; photoinduced electron transfers (solar energy conversion, charge transfer spectra of donor-acceptor systems); and biological electron transfers as in photosynthesis.

All these many branches of chemistry can be rationalized with simple theoretical ideas, for which Prof. Marcus was awarded the 1992 Nobel prize in chemistry. Such ideas include the application of Franck-Condon principle to electron transfer, that is, that the electron jumps from one ion to the other instantaneously while the ions and their associated solvent sheaths take a finite time to relax to the electron transfer. That is, the separation of electronic and nuclear motion—the nuclear configuration readjusts after the electronic transition, and not during it. Consequently the dielectric polarization of the medium cannot be treated as a continuum, the solvent molecules have discrete orientations around the ion and are changing these orientations, consequently, ideas of nonequilibrium polarization have to be incorporated into a statistical model of the jump process. To power the jump, one can consider an incident light source, however, Marcus pointed out long ago that electron transfer reactions occur in the dark and that it is thermal fluctuations in the solvent which are the driving force for the electron to jump from one ion to the other—essentially a tunnelling process which requires relatively little energy.

The theory of electron transfer also shows why electron transfer processes in photobiology must be very fast—there are numerous competing processes on a longer timescale. For example, the chromophore absorbs a photon, thereby exciting an electron. On a nanosecond timescale this excited electron can fluoresce, or it can couple to the vibrational ladder of states through a intramolecular vibrational energy transfer process and lose energy this way. Consequently, the longer the excited electron hangs around, the greater the probability that it will lose energy—energy which will not be available latter on for chemical synthesis. Within a protein molecule there is no solvent sheath so the electron transfer process is very fast—there is only an electronic component, no solvent reorganization.

Prof. Marcus concluded his talk with a discussion on the theory of electron transfer within proteins. In this theory, an artificial intelligence method has been developed for selecting the amino acids most important for the intramolecular electron transfer, for use in the calculation of the donor–acceptor electron transfer coupling factor. Such a procedure greatly reduces the computational difficulties. Experimental studies of such systems are now becoming almost routine with the technology of molecular biology. Selected site mutagenesis allows one to make proteins with donor and acceptor groups in particular places in their structure—controlling the distance over which the electron has to jump. It is found that the rate or ability of the electron transfer depends upon electron rich pathways between donor and acceptor groups.

Richard E. Smalley (Rice University, USA)
Fullerene Nanowires

We are currently hearing a great deal about molecular electronics, where chemists are synthesising and assembling new molecules which will have the

electrochemical properties of very much larger pieces of inorganic semiconducting material. However, what of future developments? One of the prerequisites of a viable nanoscale device is a means of conducting the electron from one part of the nano-device to another without it going to ground, a short circuit. That is, how do you make a nanowire?

At a molecular level, the transfer of an electron requires overlap of donor electronic orbitals with those of the acceptor. Due to the usual atomic localization of orbitals, this desired overlap is a strong function of the distance between donor and acceptor. But the overlap can be effectively extended by incorporating an intervening material which itself overlaps with both the donor and acceptor orbitals. Molecular electricians are currently seeking nano-conductors that confer structural rigidity, preventing spatial arrangements which lead to molecular short circuits.

Prof. Smalley, one of the discoverers of C_{60}, pointed out that a single graphite sheet, a graphene layer composed of carbon in a hexagonal lattice, would have an enormous tensile strength—perhaps a 100 times greater than steel, being a single molecule even though it might have macroscopic dimensions. Such sheets provide the only known example where atoms of a single element combine to produce a chemically passive two dimensional surface. If pentagons are incorporated into such a sheet it will being to assume positive curvature. With 12 pentagons, the surface closes to give a fullerene which may be either spherical (C_{60}) or tubular (nanotube).

If heptagons are incorporated into a graphene sheet, then negative curvature will be given to the two dimensional surface. Prof. Smalley outlined nanotechnologies based on the addition of pentagons and heptagons to graphene sheets to produce a variety of new materials which would be chemically resistant and very strong. He went on to outline the production of nanotubes which would have walls a single carbon atom thick (1 nm in diameter), but would be many thousands of times longer. Such tubes would be conductors, but if doped, as is done in graphite intercalates, with Na or Cs they would become exceptional conductors.

To produce these tubes has been something of a 'black art', they are produced to varying degrees with the carbon arcs used to produce fullerenes. However, the optimal conditions have only been found be trial and error. Prof. Smalley outlined a model for the optimal production. It was known that small amounts of Fe or Ni catalyzed the production of the nanotubes—how was something of a mystery. Smalley's model is that small particles of the metals attach themselves to the open end of a curved graphene sheet—preventing the cap from closing. Depending on the diameter of the metal particle, the diameter of the graphene tube and the pressure of inert gas in the arcing device a number of products are possible. If the metal particle diameter is very much greater than 1 μm and with an inert gas pressure of an atmosphere, the main product of the arcing is graphite. If the metal particles are smaller than a few nanometers and at pressures less than an atmosphere, then diamond is the main product of the arcing process. However, for metal particles slightly smaller than a micron and at pressures less than or equal to an atmosphere, carbon nanotubes are produced in large quantity. What appears to be happening is that carbon dissolves in the metal particles and precipitates out of the metal on the growing nanotube which is attached to the metal particle.

Appropriate chemical substitutions inside and/or outside these nanostructures offer an array of rationally designed new materials including semiconductors, superconductors, nanowires and catalysts.

Frank E. Karasz (University of Massachusetts, USA)

Electroluminescense in π-conjugated polymers

Prof. Karasz described the synthesis of multi-block alternating copolymers of rigid phenylene vinylene units of specified length interspersed with flexible spacer groups of methylene or of ethylene oxide oligomers. These materials are soluble and film forming, and by varying the chromophore length and/or by derivatization can be tuned to provide electro-luminescence at specified wavelengths to essentially cover the entire visible spectrum. The electrodes in a typical arrangement are indium-tin oxide and Al, Ca, Mg or Ag; the active polymer matrix is, of order, 100 nm thick and the driving voltages are about 10–30 V.

Karasz demonstrated how the luminescence varied with the nature of blends of these copolymers, and with mixtures containing other chromophorically active macromolecules. Greatly improved quantum efficiency can be obtained by adopting different configurations and incorporating electron and/or hole transport layers. Charge injection under reverse bias also leads to light emission under certain conditions and to further understanding of the photophysics of these new materials.

This Congress was not as well attended as previous IUPAC congresses, there were about 800 delegates. There was a small exhibition of industrial organizations, including the official publisher of the Union—Blackwell Science Ltd.

What was noticeable however was the strong boost this Congress has given to local or regional chemists. It was apparent that a great many of the delegates were from the Middle East and Asia, there were some chemists from the United States and Western Europe, however, they were very much in the minority.

Thirteen million – and still growing

For Chemical Abstracts Service, 1994 was a year of unprecedented database growth and improved delivery of information, IUPAC affiliate Dr W. Val Metanomski reports.

The theme for Chemical Abstracts Service (CAS) activities in 1994 might well have been 'bigger and better', reflecting both the expanded volume of information processed and the improved, more timely, accessibility on-line.

First, consider the raw numbers. During 1994, CAS abstracted and indexed 653 055 papers, patents, and other publications. This was an all time annual record well over the previous high number of 553 051 in 1991. In addition, CAS cited 122 752 equivalent patents in 1994.

An all time record was also noted in the growth of the CAS Chemical Registry System. In 1994, 777 212 new chemical substances were added to the System, again well over the previous high number of 690 313 in 1992.

CAS milestones for the year included the registration of the 13-millionth chemical substance and the publication of the 15-millionth abstract.

The 13-millionth chemical substance registration was a synthetic polymer, a novel poly(amide imide), reported in a paper by three German researchers at the University of Freiburg, H. A. Schneider, N. Steinhauser, and R. Mülhaupt (*CA* **121** (2), 10424x) (see below).

The 15-millionth *CA* abstract, published in March 1994, reported on 'Fire- and dripping-resistant resin compositions', patented by two Japanese researchers, Y. Mishima and R. Yoneyama (*CA* **120** (12),136218f).

In 1994, the largest share of the journal literature again came from USA (29.2%), followed by Japan (12.7%), Germany (6.6%), People's Republic of China (6.2%), United Kingdom (5.5%), and Russia (4.6%). The most noticeable upward change was in the number of papers originating from the People's Republic of China, from 8797 in 1984, to 14 748 in 1989, to 33 684 in 1994. The list of 192 countries, where the reported work was done, included such countries as Cyprus (9 papers), Fiji (5 papers), Grenada (2 papers), Mozambique (2 papers), Namibia (3 papers), and Samoa (2 papers).

In terms of language, in 1994, papers published in English rose to 81.9% (from 69.2% in 1984 and 73.8% in 1989), followed by Russian (5.2%), Chinese (4.6%), and Japanese (4.2%). The contributions in German showed a marked decrease (1.5%, down from 3.4% in 1984), and so did those in French (0.6%, down from 1.3% in 1984). Among lesser-known languages, within the total of 49 languages in which papers were published, are: Cambodian, Georgian, Kazakh, Sinhalese, Thai and Uzbek.

Within the 107 226 patents abstracted in 1994 (another annual record), the Japanese again had the largest share (61.0%), followed by USA (8.5%), the European Patent Office (EPO) (8.3%), and the World Intellectual Property Organization (WIPO) (8.0%). The equivalent patents cited in *CA* showed a somewhat different distribution: Japan (30.6%), EPO (20.1%), USA (13.5%) and Canada (8.4%).

With respect to changes in different chemical fields in the past five years, while the total number of abstracts increased 33.5%, the greatest increase occurred in the Applied Chemistry and Chemical Engineering Sections (41.8%), followed by that in the Biochemistry Sections (38.4%). Focusing on more specific subdisciplines, within the Biochemistry Sections, the largest increases were noted in the fields of biochemical genetics; radiation biochemistry; nonmammalian biochemistry; mammalian pathological biochemistry; immunochemistry; and fertilizers, soil, and plant nutrition.

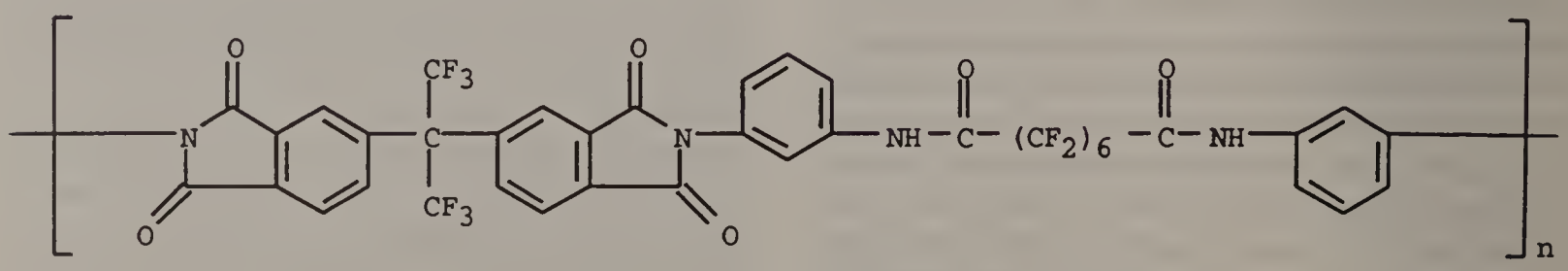

Fig. 1 Poly[(1,3-dihydro-1,3-dioxo-2*H*-isoindole-2,5-diyl)[2,2,2-trifluoro 1-(trifluoromethyl)ethylidene](1,3-dihydro-1,3-dioso-2*H*-isoindole 5,2-diyl)-1,3-phenyleneimino(2,2,3,3,4,4,5,5,6,6,7,7-dodecafluoro 1,8-dioxo-1,8-octanediyl)imino-1,3-phenylene] *[1155827-99-91]*.

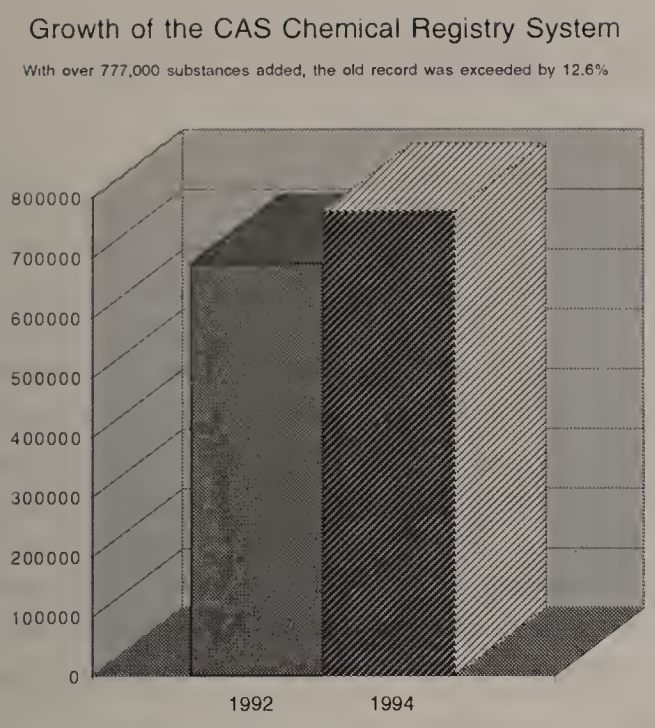

Fig. 2 Growth of the CAS Chemical Registry System. With over 777 000 substances added, the old record was exceeded by 12.6%.

Within the Applied Chemistry and Chemical Engineering Sections, the largest increases were noted in the fields of mineralogical and geological chemistry; nonferrous metals and alloys; and air pollution and industrial hygiene.

Besides providing more new chemical information than ever, CAS also began to deliver this information on-line with improved timeliness through the new CAplus database. CAplus, available on the STN International network as of January 1994, includes the comprehensive coverage already found in the CA file, but offers expanded information from 1300 key chemistry journals. For these publications, CAplus includes biographical items, book reviews, editorials, and other significant items not traditionally covered in CA.

Data entry for CAplus is completed in four to six days from receipt of the journal by CAS, making this database the most current information available. The database is updated daily, and current-awareness searchers (SDIs) can be run weekly or biweekly.

Other new services introduced in 1994 included the CAS Web Server and SciFinder, both expanding CAS's reach in the cyberspace community.

The Web Server brought the growing universe of Internet users more convenient access to information on CAS products and services, training opportunities, and news about CAS. Internet users with Web browsing software, such as Mosaic, can reach the CAS Web at http://www.cas.org.

SciFinder, a client-server product, introduced 'point-and-click' access to CAS information. With an intuitive, graphical interface, SciFinder gives scientists with no on-line searching expertise a nearly effortless way to ask the questions routinely encountered in their work – and get answers immediately from the vast resources of CAS.

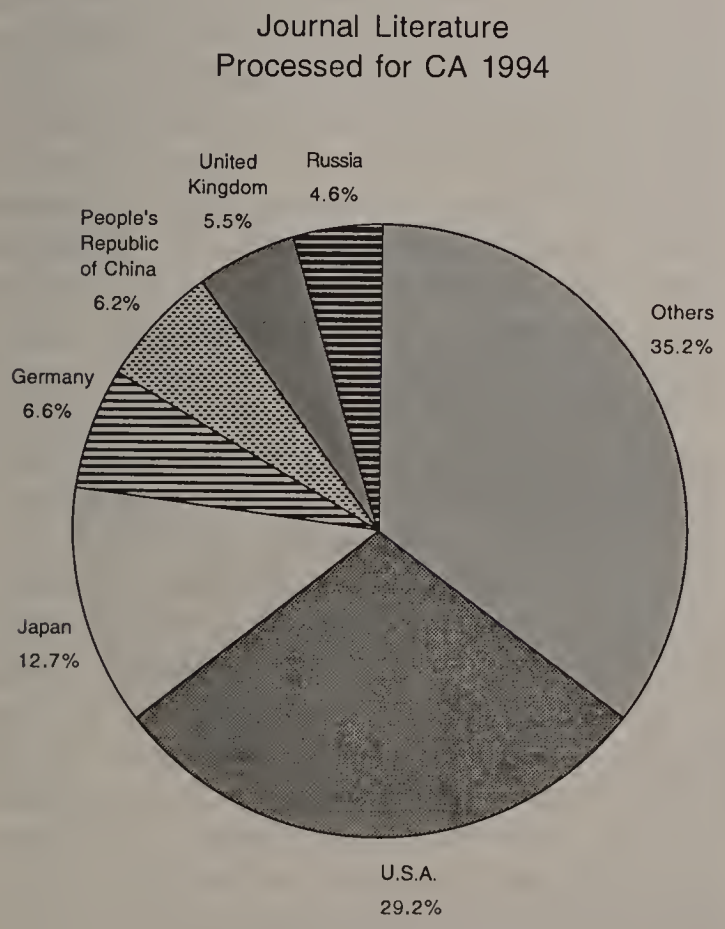

Fig. 3 Journal literature processed for CA in 1994.

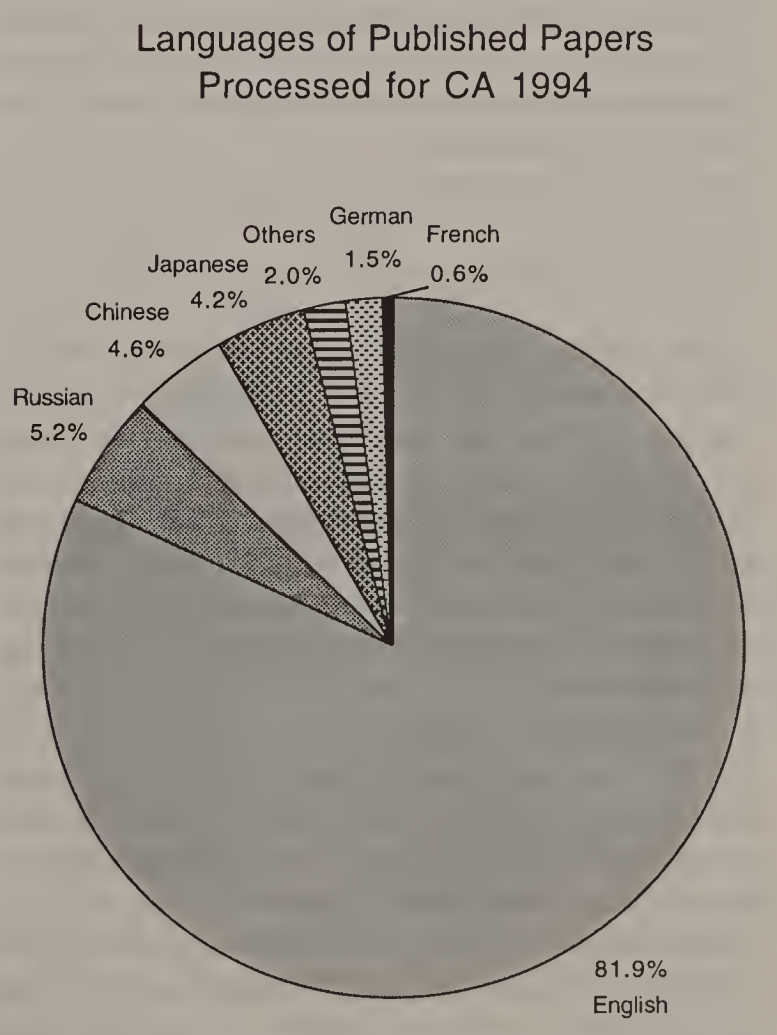

Fig. 4 Languages of published papers processed for CA in 1994.

The consequences of poor mixing

As students of chemistry, we were all familiar with simple solution-based chemical reactions. Perhaps one of the earliest examples we observed were the colour change in acid-base indicators when an excess of acid is added to a base or *vice versa*. Such colour changes occur quickly and, if the pH of the solution is not reversed, are irreversible.

There exists a class of solution chemical reactions, however, which are reversible. Indeed, are reversible on well established time scales – clock-reactions. In a clock-reaction, reactant solutions of known concentrations are mixed, and there is no apparent reaction until, after a precalculated interval – a function of the concentrations, the solution changes colour.

The prototype of such clock-reactions is the chlorite-thiosulfate reaction. In this system, it is observed that, for a certain starting concentration, for the first few minutes the measured pH of the solution increases smoothly. Then the pH is observed to fall, the time after which it starts to fall depends upon stirring rate.

Mechanistic analysis of the thiosulfate-chlorite reaction as well as considerations of the reaction-time distributions has lead to the following qualitative explanation of the observed temporal behaviour of the solutions. The pH rise, and subsequent drop, result from competition between two reaction pathways both starting from thiosulfate and chlorite:

$$4S_2O_3^{2-} + ClO_2^- + 4H^+ \rightarrow 2S_4O_6^{2-} + 2H_2O + Cl^- \qquad (1)$$

$$S_2O_3^{2-} + 2ClO_2^- + H_2O \rightarrow 2SO_4^{2-} + 2H^+ + 2Cl^- \qquad (2)$$

Reaction 1 is responsible for an initial rise in pH. Reaction 2 accounts for the fall in pH. In the bulk solution, reaction 1 is the dominant pathway. However, if in a small region a fluctuation of solute concentration leads to a sufficiently high concentration of hydrogen ions, the autocatalysis in reaction 2 can produce a rapid local accumulation of H^+ which spreads through the solution, causing the observed rapid pH fluctuation. Although such behaviour is rare, it is by no means limited to the chlorite-thiosulfate reaction.

It is one of the recent great advances in our understanding of the physical world that we have begun to become conscious of the importance of nonlinearity in dynamic systems. Linear systems, for example, a chemical change $A \rightarrow B$, are susceptible to exact mathematical analysis – the whole is the sum of the individual parts. They are, however, only a small percentage of the dynamics observed in the real world. With increasing regularity, particularly with new and continuous advances in computational power, we are seeing that science deals with nonlinear systems that give rise to complex temporal oscillations, chaos and spatial pattern formation. Such complex behaviour arise because in any system governed by a nonlinear rate law, a knowledge of the bulk or average concentrations is not sufficient to predict the average rate of reaction. One must identify the spatial distribution of solutes within the reaction vessel. The further the rate law deviates from linearity, the more drastic will be the dependence of the system on the spatial distribution of reacting species.

Autocatalysis is the enhancement in the absolute rate of a chemical change as that chemical change is occurring. The product of the reaction, or an intermediate formed during the reaction, can act as a catalyst and the rate of the reaction is accelerated – as seen in the coupling of the two reactions present in the thiosulfate-chlorite reaction above. This process of autocatalysis is very common in biological systems and has even been invoked as a mechanism for evolutionary change. In chemical systems, autocatalysis can lead to an explosion if, for example, an exothermic reaction which possess a rate that increases rapidly with temperature is run in a closed vessel that does not permit a sufficiently rapid heat lose to the surroundings.

Autocatalytic chemical reactions, when coupled to other reactions that provide a negative feedback to control the proliferation of the autocatalytic species, can produce complex behaviours such as periodic oscillations or chemical chaos. In configurations open to the flow of matter and or energy, such as stirred-tank reactors commonly used in chemical engineering, autocatalytic chemical systems can support multiple stable states, leading to hysteresis as a control parameter for the reaction is varied.

Although it might be imagined that mixing is a trivial matter of stirring the reactants together at high velocity. The assumption that a medium is 'well mixed', that is, that the concentration of reactants is uniform throughout the system, is not at all easy to achieve in practice. If the reaction under investigation is a simple first-order process, then slight departures from homogeneity in the stirred-tank reactor will not effect the final outcome. However, if the reactions are nonlinear where the overall rate of reaction is depended in a nonlinear manner on one or more reactant concentrations, any departures from perfect mixing can have major dynamic consequences and can strongly perturb the distribution of products.

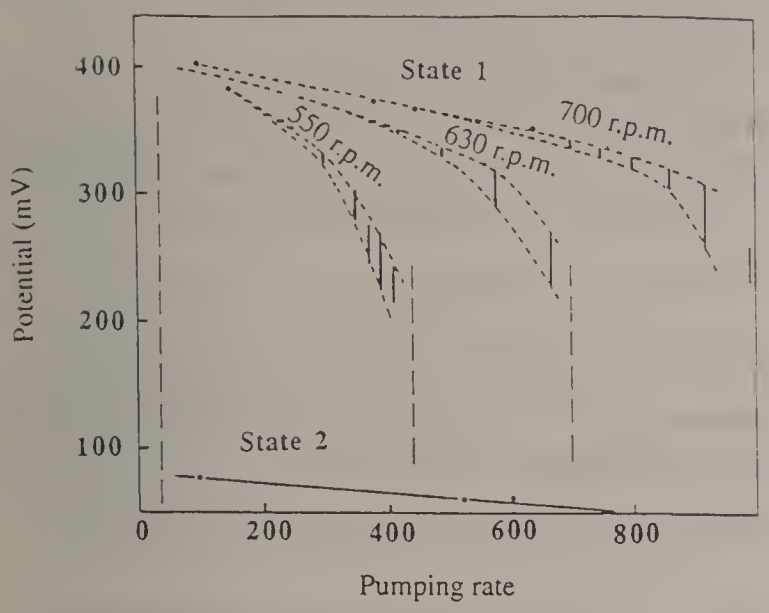

Fig. 1 Effect of stirring on the bistability observed in the chlorite-iodide reaction. Dashed line gives the steady-state potential in state 1, the solid line gives the steady-state potential in state 2. The bistable region shifts and broadens as the stirring rate is increased. (The pumping rate is given in units of 0.02 mL/min, and the potential is that of a Pt electrode vs. an $Hg/HgSO_4/K_2SO_4$ reference electrode.) Taken from I. R. Epstein, *Nature* 374, 321–327 (1995).

A perfectly mixed system is as much a theoretical concept as is an ideal gas. Chemical engineers spend a great deal of their time adjusting parameters of reaction vessels to make the contents of a reaction vessel as perfectly mixed as possible, and learning to deal with departures from perfection in mixing. Mixing is an extremely complex phenomenon, occurring on multiple time scales and length scales. Chemical engineers speak of two aspects of mixing, macromixing and micromixing. The former involves intermingling of packets of fluid, such as those that enter a reaction vessel in two streams, to achieve a composition that appears homogeneous if sampled on a macroscopic scale. Micromixing, which is a far slower process and one which is more difficult to achieve, involves segregation of a fluid in vortices and filaments at very short length scales.

From a theoretical point of view, the extreme cases of perfectly mixed, homogeneous systems and of unmixed, diffusive systems are far better understood than the commonly occurring intermediate case of partially mixed systems. An accurate model of this type of system is far beyond our current theoretical capacity, however, even a crude model, involving the coupling of standard ideal models, can give many insights into many of the phenomena of interest which are readily observed in the laboratory.

One of the first demonstrations of the importance of mixing on observed reaction products was that by Roux *et al.* (see I. R. Epstein, *Nature* **374**, 321–327 (1995) for a detailed history of this problem) on the chlorite-iodide reaction. Typical results are shown in Fig. 1. It was remarkable that the bistability and hysteresis of this system was so strongly effected by the rate at which the solution mixture was stirred.

A simple model involving two coupled stirred-tank reactors, one well stirred (well mixed) with volume V_a, and the other poorly stirred (badly mixed) with volume V_d, was invoked to explain the results, see Fig. 2. The model states that the ratio of the transition time between steady states of differing composition to the residence time (inverse of flow rate) in the reactor that determines how changing the degree of mixing will influence the stability of the two bistable branches of the steady states. Varying the stirring rate in such coupled reaction vessels can favour reactions branches which occur more readily in slow moving or faster moving sections of the fluid.

It was observed that a Pt microelectrode placed at various distances from the central stirring rod in a chlorite-iodide reactor gave very different readings for particular stirring rates. In one case, at a stirring rate of 880 r.p.m, a factor 8 difference in the concentration of iodide was observed in measurements on axis and 12 mm away in the radial direction in a cylindrical reactor. Even at rates of 2820 r.p.m., just below the threshold for cavitation, iodide concentration differed by 17% between the axis of the reactor and the tip of the stirrer.

One of the most famous of such complex oscillating solution reactions is the Belousov-Zhabotinsky reaction (BZ). In 1958, Belousoz reported an oscillatory reaction in an originally homogeneous solution, namely, the oxidation of citric acid by potassium bromate catalysed by a cerium ion redox system (Ce^{3+}/Ce^{4+}). Zhabotinsky in 1964, examined this reaction and showed that similar phenomena occurred with malonic acid and also with other catalysts. The malonic acid is oxidized by the bromate to CO_2 and formic acid. The reaction network includes a number of intermediate stages in the reduction of bromate and there are two reaction pathways, one requiring high bromide ion concentrations and the other the autocatalytic production of bromous acid with the aid of Ce^{3+} ions. Both of these ions are products of the final oxidation step, so there is positive feedback on the two alternative pathways, which are operative when $[Br^-]$ is high and when it is low. Indeed, the two-reactor model displayed in Fig. 2 has played a major role in unravelling the mechanism of the BZ reaction. It was discovered that the observed chaotic chemical behaviour in the BZ reaction came not from the inherent homogeneous chemical kinetics of the system, but from the coupling of those nonlinear rate laws with imperfect mixing conditions in the experiment.

Such complex coupled nonlinear chemical reactions, far from equilibrium, may evolve in unexpected ways

and reveal the necessity of theoretical models involving network analysis – models much more complex than those usually used for modelling linear chemical reactions. The BZ reaction is an example of what Prigogine, and the Brussels school, call a dissipative structure, that is, an open system through which matter and energy flow and which maintain inhomogeneity and order, or rather, organization at positions far removed from equilibrium.

As a physical example of such a system, consider a heated column of fluid. Eventually, a continuous small gradation of temperature is created with the hotter fluid nearer the source of heat. As the heating continues, the temperature gradient rises, until at a critical value (Bénard instability point) internal convection occurs spontaneously where large domains of fluid move in a concerted manner. This highly cooperative motion can display a spatial regularity, in the form of cells of fluid. The energy of random thermal uncoordinated fluctuations of molecules in the fluid has been, at least in part, replaced by the energy of cooperative macroscopically ordered motion. The probability of such a process occurring spontaneously through random motion at equilibrium, from the Boltzmann principle, is vanishingly small; an external constraint, the thermal gradient, has apparently been able to drive the system sufficiently far from equilibrium so as to create an ordered structure in the fluid. This is a nonbiological example of what Prigogine would term *order through fluctuations.* A new structure has arisen from an instability, a random stochastic element, viz a fluctuation which at a critical point, can be amplified and allow a new structure which replaces a pre-existing structure. It is the nonlinear character of the relation between flows and forces which is the necessary condition for order to arise through fluctuations. Physical examples of such systems are rare, however, chemical networks have an almost unlimited variety and complexity, and moreover, are often nonlinear in character and not close to equilibrium.

An example

We are familiar with the standard models of linear kinetics. But to consider what happens when some nonlinearity enters the kinetics of a reaction, consider a set of species with populations c_1, c_2, ... Assume that each increases and decreases at rates proportional to their population,

$$(dc_i/dt) = (b_i - d_i)c_i = r_i c_i$$

where b_i and d_i are the rate of increase and rate of lose, respectively, with r_i being the net growth rate of the ith species. If reactants are in plentiful supply and there are no additional reactions consuming products or reactants, then all populations will grow exponentially and the species with the largest growth rate will come to dominate the final population distribution regardless of initial populations, c_{i0}.

If the initial populations of two components are coupled, that is, we constrain the total population, $C = \Sigma c_i$. If we take, for example, initial populations c_{10} and $c_{20} = C - c_{10}$ the growth or rate equations become

$$(dc_1/dt) = r_1 c_1 - (c_1/C)(r_1 c_1 + r_2 c_2)$$

$$(dc_2/dt) = r_2 c_2 - (c_2/C)(r_2 c_2 + r_1 c_1)$$

Because $(dc_1/dt) + (dc_2/dt) = 0$ and $c_1 + c_2 = C$, we can obtain a single rate equation for c_1:

$$\begin{aligned}(dc_1/dt) &= r_1 c_1 - (c_1/C)[r_1 c_1 + r_2(C - c_1)] \\ &= [(r_1 - r_2)/C][c_1(c_1 - C)]\end{aligned}$$

which when solved yields for $c_1(t)$ – the temporal evolution of reactant c_1

$$c_1(t) = C/[1 - (1 - C/c_{10}) \exp[(r_1 - r_2)t]]$$

where as $t \to \infty$ the expression for $c_1(t)$ approaches zero if $r_2 > r_1$; it approaches C if $r_2 < r_1$. We thus have an 'all or nothing' selection of the faster growing concentration,

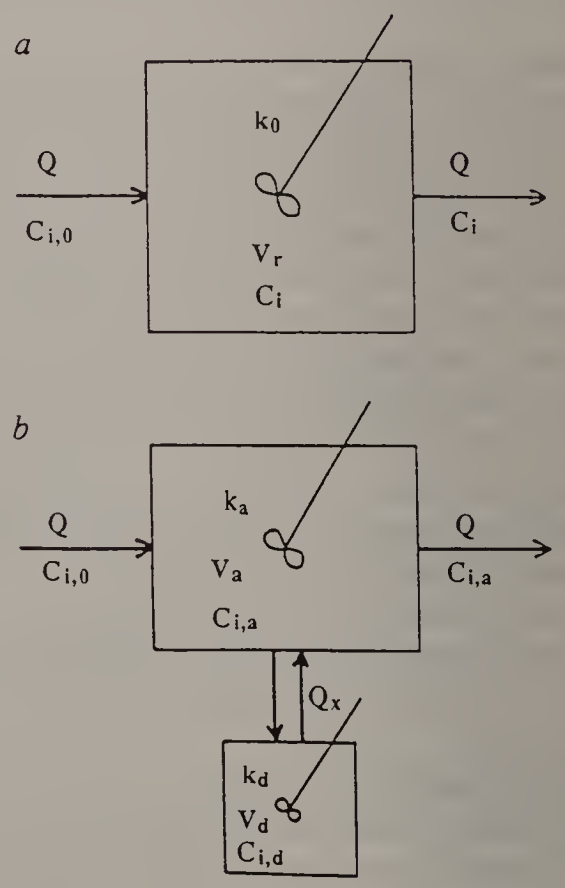

Fig. 2 Two-reactor model of imperfect mixing in a stirred-tank reactor. (a) An idealized system in which mixing is perfect with homogeneous concentrations throughout. (b) Stirred-tank with cross flow into a poorly stirred (poorly mixed) volume. *Q* is the volume flow; *C*, the concentration; *k*, the flow rate; *V*, the volume; chemical species are represented by subscript *i*, *o* representing input values; *r*, homogeneous reactor, a and d represent the active and dead zones, respectively). Taken from I. R. Epstein, *Nature* 374, 321–327 (1995).

independent of the initial conditions, so long as neither starts at zero.

Consider now a pair of concentration species evolving with a nonlinear growth rate, for example, quadratic. The evolution or rate equations for the system now take the form

$$(dc_1/dt) = r_1c^2_1 - (c_1/C)(r_1c^2_1 + r_2c^2_2)$$

$$(dc_2/dt) = r_2c^2_2 - (c_2/C)(r_2c^2_2 + r_1c^2_1)$$

Again making the constraint substitution, $C = \Sigma c_i$, algebraic manipulation yields,

$$(dc_1/dt) = -[(r_1 + r_2)/C]c_1[c_1 - r_2C/(r_1 + r_2)](c_1 - C)$$

Analysis of this equation reveals that if c_1 is initially less than $c' = r_2C/(r_1 + r_2)$ it will decrease until it reaches a final value of zero, that is, species 1 will disappear. If $c_1 > c'$, then it will grow until it reaches C. Again, we have an all or nothing selection of the two concentrations, but now the successful species, that species which will dominate the final product distribution, depends, not simply on the growth rate, but on whether or not c_1 initially exceeds c'.

To make an analogy with evolutionary processes, survival of the fittest is no longer the operative principle, it matters who gets in first – who starts off with the most appropriate concentration or population. Selection that is dependent on the initial conditions occurs for any growth law that exceeds linearity in its dependence on the concentrations.

The Committee on Teaching of Chemistry (CTC): an appraisal

Krishna V. Sané

The Committee on Teaching of Chemistry (CTC) was set up as a Standing Committee by IUPAC in 1964 (when Lord Alexander Todd was IUPAC President) with Professor Sir Ronald Nyholm as the first Chairman and Dr. Peter Sykes as the first Secretary.

To begin with, CTC consisted of eight members nominated by the IUPAC President from international education circles. From 1987, to facilitate CTC interaction with other Divisions, eight additional members have been nominated by Analytical, Applied, Clinical, Inorganic, Macromolecular, Medical, Organic and Physical Divisions. In addition to the 16 Titular Members, IUPAC member countries appoint National Representatives (NR) through their National Adhering Organizations. At present, CTC has about 25 NRs from as many countries.

The terms of Reference of CTC are:

1 To advise the President and the Executive Committee on educational matters.

2 To coordinate the educational interests and activities of all IUPAC bodies.

3 (a) To act as an international and coordinating body for Chemical Education throughout the world and:

(i) to establish a system of National Representatives as a channel of communication,

(ii) to develop liaison with international organizations such as UNESCO,

(iii) to develop liaison with national Chemical Societies or Chemical Education Committees.

3 (b) To promote workshops on educational problems, particularly in developing countries.

Programmes

The various CTC activities can be broadly classified as Conferences, Workshops and Publications.

Conferences

The biennial International Conferences on Chemical Education (ICCE) held since 1971 in different parts of the world have become one of the most eagerly awaited events on the CTC calendar. An ICCE, typically attended by about 600–700 delegates from 70–80 countries, consists of Plenary lectures (usually featuring one or more Nobel Laureates), poster papers, 'birds-of-feather' sessions, and Symposia/Workshops on special themes. These Conferences have done much to bring together researchers and teachers from different regions and different levels. The last ICCE, No. 13 in the series, was held in August 1994 at the Inter American University in San Juan, Puerto Rico, while the next ICCE is scheduled for 16–20 July 1996 at the University of Queensland, Brisbane, Australia. The 15th ICCE will be held in Cairo, Egypt, in 1998.

In view of the fact that participants from developing countries are under-represented at the ICCEs, it may be useful in future to explore if CTC can sponsor Regional Conferences on Chemical Education (RCCEs) in

specific regions such as Asia, Africa, South America and so on. A Regional Conference will have a format similar to an ICCE; it will also have an international character as far as presenters (i.e. speakers, workshop leaders, etc.) are concerned. But a RCCE—to be held in years alternate to an ICCE—will differ by emphasizing regional issues and regional participation. It may be added that the Federation of Asian Chemical Societies (FACS) is already deliberating on this matter and CTC could assist such efforts if a tangible proposal emerges.

Workshops

CTC, in collaboration with UNESCO, has been making a special effort to encourage teaching of hands-on chemistry in student laboratories, especially in the developing countries where the *chalk and talk* method tends to dominate the teaching/learning process. This effort has taken the form of Workshops the first being in Seoul, South Korea, in 1975 for the Southeast Asia region. College and university teachers were brought together to test and devise experiments which can be implemented under the sometimes very difficult conditions under which they have to work (e.g. lack of basic facilities, few resources, large classes, inexperienced teachers). The initial workshops, however, revealed that hands-on chemistry cannot be initiated, let alone sustained, in third world countries unless and until cost-effective solutions are found to be the problem of equipping fund-starved student laboratories with instruments, chemicals, glassware and other items required to run a meaningful teaching laboratory. The first step in this direction was the formulation of the Locally Produced Low Cost Equipment (LPLCE) Project with the following objectives.

- to develop reliable, low-cost, locally produced equipment that is easy to fabricate and easy to maintain;
- to find experiments compatible with the equipment that illustrate the principles and practice of modern chemistry;
- to transfer the know-how to teachers through hands-on workshops, manuals and videotapes;
- to set up a production unit which can supply kits and assembled equipment without a significant escalation of cost;
- to encourage curriculum changes that ensure that the whole package enables a student to be better trained for a career in chemistry.

The LPLCE Project was initiated by CTC and UNESCO in 1979 at the University of Delhi through an informal voluntary group, now known as the Edutronics Group. The 15-year old project has successfully established that a variety of solutions are possible for modernizing student laboratories using locally available materials and components.

The UNESCO-sponsored Workshops held outside of India have led to the formation of Core Groups in various countries/regions who are adapting the Delhi designs to suit local needs. UNESCO has now set up an International Network, with headquarters at Delhi University, to coordinate the activities of the Core Groups, spanning five languages (English, Portuguese, French, German and Spanish) and operating in Brazil, France, Germany, Jordan, Puerto Rico and the Philippines. The Network has established an Equipment Bank for the South Asian Countries (excluding India) which will organize: (a) training courses in fabrication, use and maintenance, and (b) supply of low-cost equipment and spare parts to institutions desirous of using such equipment.

Fig. 1 Prof. K. Sané giving instruction at the Edutronics Group Workshop held in Ljubljana, Slovenia, in 1985.

The outstanding success of the CTC/UNESCO Workshop format for popularizing the hands-on approach in the area of Low-Cost Equipment suggests that the scope of this programme be extended beyond the LPLCE activity. Inasmuch as the teaching of any subject has at least three facets: (a) content, (b) methodology, and (c) tools, it will be useful if the Workshop activity can span all three facets. Some trials have been conducted in this direction. For example, Workshops have been held on curriculum development (Berkeley, USA, 1989; York, UK, 1991; Überlingen, Germany,

Fig. 2 Students at the Edutronics Group Workshop held in Überlingen, Germany, in 1992.

1992) and on Distance Education in Chemistry (Delhi, India, 1993; Heerlen, Netherlands, 1994). Extension of LPLCE to cover other cost-effective techniques like small-scale chemistry, computer simulation and interfacing, recycling glass-ware, low-cost sensors, etc., were included in a trial CTC/UNESCO Workshop at Delhi in December 1994.

All the exploratory Workshops referred to above have emphasized a common theme, namely the teaching of environmental chemistry. An interesting outcome of these trials is the attempt to join the tools (e.g. cost-effective approaches) with methodology (e.g. Distance Education) for teaching a curriculum theme (e.g. Environmental Chemistry). This linking is taking shape in the form of a low-cost sample package consisting of: (a) some portable instruments (e.g. colorimeter and pH meter), (b) a small-scale glassware/plasticware chemical kit, (c) a multimedia unit comprising simulation, interfacing and text, and (d) printed material. The package will deal with selected aspects of the Environment like experiments with water/soil/air, simulation of the greenhouse effect, multimedia presentation of ozone depletion, etc. This test exercise, supported by ICSU and undertaken in collaboration with the Open University, UK, is intended for trials in distance education and self-learning courses as well as in conventional class-room situations. The feedback should allow a systematic strategy for preparing teaching packages on topical themes like energy and environment and also on traditional curriculum themes like chemical reactions, chemical equilibrium, chemical architecture, etc.

Publications

CTC started publishing the *International Newsletter on Chemical Education* (INCE) in 1974 to promote the exchange of ideas and the dissemination of information on chemical education all over the world. The circulation of INCE varies between 3000 to 4000 and it is printed twice a year.

CTC has produced several surveys. Some examples are: *Introduction of SI Units in School and University Teaching: Implementation and Difficulties, Survey of Chemical Education in Developing Countries*, and *Survey on Continuing Education of Chemists in Industry*. An anthology, *Chemical Education in the Seventies,* published by CTC in 1980, contains contributions from individuals in 40 countries and outlines developments in chemical education in schools, colleges and universities.

CTC has published the Proceedings of every ICCE. Many of the Workshops of the Edutronics Group have led to publications which were integrated in the form of a book *Locally Produced Low Cost Equipment for Teaching of Chemistry*. The first edition of this book appeared in 1991, the second in 1994. A companion volume *Experiments Using low Cost Equipment*, due for publication in 1995, describes over 100 experiments from pure and applied chemistry which have been standardized by teachers all over the world using the LPLCE equipment.

One of the CTC's decisions during the Hamburg meeting in 1991 was to publish a series of Resource Books in Chemistry for the benefit of teachers and students. This decision is taking shape in the following forms:

- *Selected Papers in Chemical Education Research* by R.B. Bucat & P.J. Fensham. This volume is a model for a Resource Book which is a collection of outstanding reprints in a given area. The selection of papers and the commentary are entrusted to one or more experts in the area.
- *Classics in Coordination Chemistry* by George B. Kauffman. This is not a new book but a reprint of the original title published by Dover Publications Inc. This publication has become possible thanks to the permission granted by Dover and the acceptance of our request by the author to include additional material for the CTC edition.
- *Modern Experiments for Introductory Chemistry* by H.A. Neidig & W.J. Stratton. This book is reprinted with the permission of the Division of Chemical Education of the American Chemical Society for restricted distribution in Third World countries. The original volume, compiled from papers appearing in *the Journal of Chemical Education*, was published in 1989.
- *Environmental Chemistry through Experiments—A practical approach*. This book is the English translation, organized by CTC, of the German book *Umwelt Chemie im Experimente—Ein Praktischer Leitfaden* written by H.J. Bader (the German National Representative on CTC) and R. Blume.

Details about each publication are given below.

A follow-up of the current Publication Programme should not be difficult. For example, it is hoped that the Bucat-Fensham volume will inspire (and provoke!) other CTC Members and NRs to compile suitable titles in their area of expertise. Individuals specializing in chemical education research have a special responsibility since they can assist CTC to become a focal point for encouraging work in this area and for disseminating important findings. Such a CTC initiative will be of great value to teachers who wish to base their efforts on 'tested' approaches rather than rely on intuition or 'hit and miss' schemes.

The Kauffman volume can catalyse collaborative projects with other Divisions/Commissions and lead to very useful Resource Material on (say*) The Chemical Bond*, *Chemical Equilibrium*, *Chemical Dynamics*,

Chemical Architecture, etc. Incidentally, Prof. Kozo Kuchitsu, Chairman, ex-President of Physical Chemistry, has informed the author that the Chemical Society of Japan has published (in Japanese) between 1975–1988 eighteen volumes of Source Papers in chemistry. These volumes have a format quite similar to that proposed by the CTC.

Appraisal

The 18-year association of the author with CTC has taken a variety of forms. It began with the initiation of the Low Cost Equipment Project at Delhi University. The 'outsider' status of the initial period changed to observer status (1979–81), then NR for India (1981–85), followed by Secretary (1986–90) and finally Chairman (1991–95). This wide spectrum of interaction has provided a multidimensional view of CTC which hopefully will permit an objective appraisal of the Committee, highlighting its strength and weakness and identifying some possible directions for the future.

Any assessment of a Committee like CTC has to note some of the constraints under which the Committee operates. One of these is the manpower (and womanpower) factor. Though in principle the Committee can seek help from anywhere—the LPLCE Project was initiated by an outsider—in practice even most of the NRs and Members are able to devote only a nominal time to Committee activities because of other commitments. One way to overcome this problem is to make Projects and Membership more compatible (i.e., if Projects are first identified, then members are chosen who can pilot them or vice versa). Another way is to tap the vast expertise available in various IUPAC Divisions/ Commissions. Two on-going examples which illustrate this point are:

- CTC and the Commission on Toxicology (VII.4) of the Clinical Chemistry Division are collaborating to produce a *Glossary Of Terms Used In Toxicology—An Educational Guide For Chemists*. The draft—prepared by Dr. H. G. J. Worth (nominee of the Clinical Chemistry Division on the CTC) and Dr J. H. Duffus—is being circulated to obtain feedback which will be incorporated in the final document to be published in the near future.
- CTC is participating in the IUPAC sponsored Student Oriented Nomenclature Book Project directed by Prof. C. J. H. Schutte. There is a possibility that when the CTC sponsored work on Recommendations for Definitions, Terms, Symbols and Representations in Chemistry Teaching directed by Prof. John Bradley (who is CTC's nominee on the Schutte Project) is published, the two publications may be formally linked (say) as Part A and Part B. This seems a useful idea since requirements of good teaching begin—rather than end—when the nomenclature in a particular area has been standardized.

The other limitation is the lack of funds. During the relatively affluent pre-1988 period, IUPAC allocation used to be comfortably adequate for holding eight-member meetings and provide partial support to INCE. Major CTC activities such as ICCEs and LPLCE could be organized through UNESCO support which was also available for a variety of CTC publications including INCE. The problem facing CTC now is that since 1992 UNESCO is finding it increasingly difficult to support CTC.

The experience of three decades shows that CTC can be very effective on the international chemical education scene if it opts for a catalytic role. Two striking illustrations of this statement are (i) the ICCEs and (ii) the Locally Produced Low Cost Equipment Project. In both cases, CTC conceived the idea, made a small beginning with financial support from UNESCO and planted the seed in different regions of the world. The fact that ICCEs as well as LPLCE are now flourishing without CTC/UNESCO support shows that CTC correctly diagnosed a spontaneous process and made it operational by lowering the activation energy through conceptual, organizational and funding inputs. *The International Newsletter on Chemical Education* (INCE), on the other hand, is struggling for survival because it started as a CTC responsibility and has remained so even after two decades. In the 1970s and 1980s, INCE had few problems when UNESCO support was generous and assured (and CTC budget was also adequate), but with UNESCO facing a resource crunch and CTC funds shrinking, INCE is living not because it is healthy but because of the willpower of some individuals who did not wish to write the obituary of the Newsletter during their term of office.

An exercise in self-reliance

It has been pointed out earlier that the LPLCE Project at Delhi University has five objectives:

- to develop reliable, low cost, locally produced equipment that is easy to fabricate and easy to maintain;
- to find experiments compatible with the equipment that illustrate the principles and practice of modern chemistry;
- to transfer the know-how to teachers through hands-on workshops, manuals and videotapes;
- to set up a production unit which can supply kits and assembled equipment without a significant escalation of cost;
- to encourage curriculum changes that ensure that the whole package enables a student to be better trained for a career in chemistry.

The first three objectives are being tackled under CTC/UNESCO auspices. The remaining two are the

focus of the Indian component of the Delhi University Project supported by various Indian agencies, particularly the Department of Science and Technology (DST), New Delhi, and the University Grants Commission (UGC), New Delhi. Under DST auspices, the CTC/ UNESCO prototypes have been redesigned to meet the requirement of chemistry teaching at: (i) senior secondary level, (ii) college level, and (iii) university level, and also to meet the requirements of mass production. A heartening feature of the Indian Project is the involvement of disadvantaged persons in the manufacturing/ marketing of the low-cost equipment. A country-wide teacher training programme has been simultaneously launched by UGC to train over 1500 teachers from 600 colleges in the fabrication, use and maintenance of the low-cost equipment followed by a supply of a package of equipment to the colleges to upgrade their student laboratories. It is felt that a coupling of a low-overhead production mechanism with a large-scale teacher training programme will initiate a process that will hopefully help to solve the well-known 'chicken and egg' problem in the Third World, namely: How can laboratory curricula be upgraded unless equipment, apparatus, glassware, software, etc. are available locally at *locally* affordable prices? likewise, how can such items be produced at lower prices unless curricula are upgraded to create a mass demand for the items?

By keeping the selling price only 15–20% above the cost price, the manufacturing unit has had a turnover of USD 100 000 in two years; about 300 colleges have upgraded their chemistry laboratories; DST and Delhi University have shared a 5% royalty which has been recycled to the R&D group; and 15 individuals are earning their livelihood with dignity and confidence. There seems little doubt that a model which joins technological innovation with social service and commercial viability can be a self-sustaining and self-evolving force for changing the educational pattern in countries with limited resources.

The experience of the Publication Unit of the Delhi University Project seems even more promising. Organized to overcome the absurd situation that the documentation describing low-cost developments cannot be published through the normal channels involving high cost, the Unit began by training disadvantaged women for self-employment through Desk Top Publishing (DTP). The hands-on training is provided by the preparation of educational material. Thanks to the generous donation of the hardware and software by international and national agencies, overhead costs have become manageable, thereby allowing the publication of useful educational material at spectacularly low price. (For example, a 250 page monograph with 117 illustrations has been produced in two colours for USD8.00, which is less than the cost of air-mailing it to Europe!).

The entire CTC Publication Programme (1991–95), along with the publication of the INCE issue Nos 36–44, has been undertaken by the DTP Unit. The encouragement received from various agencies is helping to make the Unit self-reliant. For example, the Federation of Asian Chemical Societies (FACS) and the South African Chemical Institute have ordered 100 copies each of the book *Modern Experiments for Introductory Chemistry* at USD5 per copy (including postage). The Royal Society of Chemistry, UK, has ordered 1000 copies of *Selected Papers in Chemical Education Research* at USD5 per copy (including postage). The Indian edition of the monograph on Low-Cost Equipment, used as a textbook for the teacher training programme, has become a best seller because of its extremely modest price.

In view of the considerable promise of the developments described above, it is suggested that IUPAC, CTC and UNESCO should consider how to institutionalize these informal and exploratory forays at combing educational and social objectives with financial self-sufficiency. The two weak links of the Delhi University Project are:

(a) its ability to attract industry as a partner;

(b) lack of professional international level quality in its products (e.g. equipment, monographs, etc.).

If these two deficiencies—which are interlinked—are removed, the CTC/UNESCO/ DST/UGC model can become a potent influence on science education in the Third World. In this context, it may be worthwhile to examine if this model's programmes can be adopted and adapted by the new ICSU Committee on Capacity Building because one of the most far reaching methods of capacity generation is to encourage local innovations and local initiatives in improving science and technology education at the grass-roots level. At an academic level this requires integrating R&D with teacher training and curricular reforms; at the non-academic level it requires collaboration between international agencies, industry, governments, and social and voluntary orgnizations.

Acknowledgements

A Ciba Foundation travel grant and an invitation to deliver a Plenary Lecture at the Ljubljana International Conference on Chemical education in 1977, marked the beginning of my association with CTC which has been rewarding and fulfilling. It would be appropriate to acknowledge all those individuals who have contributed to this enriching experience, but the full list is so long that it cannot be compressed here.

Some CTC publications

Locally Produced Low-Cost Equipment for Teaching of Chemistry (2nd edn, 1994) K.V. Sané,

D.C. West, (243 pp.) Price: USD20.

The monograph describes the fabrication, use and maintenance of three instruments (a pH meter, a conductometer and a colorimeter) having widespread utility for student level laboratory work in chemistry. Also described are the fabrication of two test instruments (a continuity tester and a OVA source which are useful either for trouble-shooting or for calibration) and of several accessories such as a magnetic stirrer, a zero-cost electrode for pH measurements, and a conductance cell. Brief theoretical sections in electronics and in chemistry are included to make the presentation self-contained. No previous experience in instrument fabrication is assumed; practical techniques such as soldering, PCB making and circuit board assembly are consequently described in detail. The monograph is liberally illustrated and uses a highly visual style in which constant reference is made to the figures.

The equipment described in the monograph has been developed under the project entitled *Low Cost Equipment for Chemical Education* sponsored first by IUPAC, CTC and UNESCO and then by the Indian Department of Science and Technology (DST) and by the Indian University Grants Commission (UGC). Valuable assistance has also been received from the International Development Research Centre (IDRC), ICSUCTS, and from the Commonwealth Foundation. The immediate aim of the Project is to develop teaching-oriented instruments for chemistry which are simple, reliable, inexpensive, easy to fabricate and easy to maintain. A wider aim is to influence the laboratory teaching in developing countries by making it more purposeful, exciting and innovative. The know-how developed under the Project is, therefore, being disseminated through hands-on teacher training Workshops. 25 such Workshops have been held outside India in every continent under the auspices of UNESCO while 35 Workshops have been organized all over India under the sponsorship of UGC.

Partial contents:

Part (i) Theoretical aspects

Part (ii) Electronic components and circuits

Part (iii) Assembly of instruments and accessories

Part (iv) Principles of circuit operation, calibration, use and maintenance of the instruments

Part (v) Experiments using the low cost instruments

Bibliography

Modern Experiments for Introductory Chemistry.
H.A. Neidig & W.J. Stratton, (135 pp.) Price: USD5.

The first edition of this book was published in 1967. A revised and updated volume was published in 1989. The low-cost CTC Edition has been published by arrangement with the Division of Chemical Education, American Chemical Society. It should be noted that the CTC and the Publisher are granted distribution rights worldwide, except for the following areas: North American Free Trade Area, European Union (Common Market), Japan, Australia and New Zealand. Sales may not be made nor orders accepted from addresses within these areas. Sales of single copies are permitted at ICCE meetings to participants. Sales of single copies are permitted to individuals with addresses in Mexico, but not to corporations or booksellers. This is a specific exception to the North American Free Trade Area.

Excerpts from the preface

'In the 20 years since the appearance of the first edition, a great many articles have appeared in the *Journal of Chemical Education* describing interesting new laboratory experiments. We have assembled here a selection of what we think are among the best articles from the last 20 years along with a moderate number of articles retained form the first edition. Our goal has been to select experiments that will appeal to instructors who are looking for new ideas. We remind the reader that many excellent laboratory manuals exist and that several publishers offer a wide range of experiments in modular form. For the most part, we have rejected the cut-and-dried illustrations of concepts. We have favoured experiments that require thinking, for which there may be an element of challenge, and where there will frequently be a genuine unknown for the student. It is this problem-solving approach that we assume to be at the heart of science. With this in mind, we have included a few provocative articles form the *Journal* that discuss pedagogical issues of laboratory teaching.

One noteworthy development since the appearance of the first edition has been the widespread interest in project laboratory programs, which occupy anywhere from several weeks to a whole semester. We think these have much to commend them for those instructors willing to invest the effort in their planning and implementation. We have included a selection of project experiments.

We have limited our selection to experiments that can be done with the equipment normally now available for use in first-year college chemistry courses. This included pH meters and simple spectrophotometers, but no IR, NMR, GC or HPLC. Some otherwise excellent experiments have been eliminated for this reason. We have also been guided by safety considerations and have regretfully eliminated a number of good experiments because they require use of chemicals that are now recognized as being unusually hazardous to human health.

We have included a few editorial comments, especially calling the attention of the reader to other related articles that have appeared in the *Journal*.'

Partial contents

Properties

BASIC and the density of glass [1986, 63, 718], A.D. Harris.

A CO_2 soap bubble dynamics [1978, **55,** 807], R.C. Millikan.

A simple experiment of determining vapor pressure and enthalpy of vaporization of water [1982, **59,** 337], G.S. Levinson.

Is volume conserved? [1986, **63**, 538], John Olmsted, III.

Experiments with butane lighter fluid [1976, **53,** 306], D.A. Davenport.

Stoichiometry

Simplest formula of copper iodate: a stoichiometry experiment [1983, **60,** 147], D.J. MacDonald.

A continuous variation study of heats of neutralization [1981, **85**, 730], D.W. Mahoney, J.A. Sweeney, D.A. Davenport, R.W. Ramette.

A simultaneous analysis problem for advanced general chemistry laboratories [1983, **60,** 673], J.J. Leary, T.N. Gallaher.

Kinetics

Oxidation of ethanol by chromium (VI) [1971, **48**, 473], M.E. Finlayson, D.G. Lee.

The reactions of ferroin complexes [1975, **52,** 408], J.O. Edwards, K. Edwards, J. Palma.

Kinetics of oxidation of bromocresol green [1987, **64,** 81], M. Pickering, D. Heiler.

The colour blind traffic light [1972, **49,** 312], J.F. Lefelhocz.

First-order decomposition of the violet coloured Ce(IV) oxidation product of n-phenylanthranilic acid [1976, **53**, 327], S.K. Mishra, P.D. Sharma, Y.K. Gupta.

Equilibrium

Silver equilibria via cell measurements [1972, **49**, 423], R.W. Ramette.

The solubility of $CaSO_4$: an ion exchange-complexometric titration experiments for the freshman laboratory [1976, **53**, 254], E. Koubek.

Conjugate acid-base mixtures in the general chemistry laboratory [1978, **55,** 401], G.R. Wiger, U. de la Camp.

Determination of pKa using the half-volume method [1977, **54,** 711], S.J. Stephens, M.J. Joncich.

Thermodynamics

An inexpensive voltaic cell [1978, **55**, 50], T.L. Miller, J. DiPaolantonio II.

A Gen Chem thermodynamics experiment [1978, **55,** 53], C.L.P. Beaulieu.

A thermochemistry experiment for freshman lab [1985, **62**, 172], D.P. Miller.

Thermochemistry of hypochlorite oxidations [1965, **46,** 378], M.J. Bigelow

Thermodynamics and solubilities of salts of dipositive ions [1979, **56**, 206], G.F. Riley, W.H. Eberhardt.

An individualized Nernst equation experiment [1985, **62,** 875], G.F. Hambly.

Qualitative analysis

A thin-layer chromatography experiment for general chemistry [1970, ***47***, 401], S. Lincoln, S.H.C.J., R.A. Pohl, D.T. Haworth.

Ion exchange chromatography and spectrophotometry [1985, **62,** 170], N. Foster, B. Pestel, B. Mease.

Quantitative analysis

Vitamin C and the diet of a student [1972, **49,** 738], J.E. Fulkrod.

An introductory quantitative laboratory exercise [1977, **54**, 190], A.J. Crossfield.

Titration of calcium and magnesium in milk with EDTA [1973, **50**, 136], P.G. McCormick.

The determination of calcium in dietary supplement tablet by ion-exchange [1986, **63,** 177], M.L. Dietz.

The determination of copper in a copper-nickel alloy [1978, **55,** 660], K. Gallagher, C.R. Cantor.

Determination of phosphoric acid in cola beverages [1983, **60,** 428], J. Murphy.

Vitamin C content of commercial orange juices [1977, **54**, 192], P. Haddad.

Determination of the percent Na_4EDTZ in bathroom cleaners [1978, **55,** 265], K.I. Kump, F.A. Palocsay, T.N. Gallaher.

Bicarbonate in Alka-Seltzer [1980, **57**, 517], L. Peck, K. Irgolic, R. O'Connor.

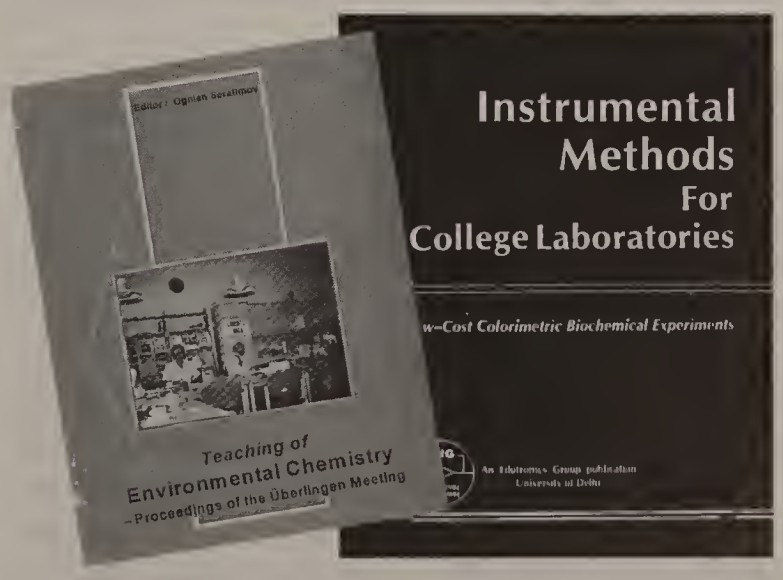

Fig. 3 Some of the above publications.

An experiment in forensic chemistry: the breathalyzer [1986, **63**, 897], W.C. Timmer.

Reactions and synthesis

A simple oxidation-reaction experiment [1976, **53,** 377], S. Marie Ludeman, J.A. Brandt, G. Zon.

Ion exchange separation of the oxidation states of vanadium [1980, **57,** 316], R. Cornelius.

The science and magic of chemistry: a learning cycle laboratory on oxidation-reduction [1986, **63,** 1098], R.G. Silberman, A.P. Zipp.

Investigation of some metallochromic indicators [1979, **56,** 755], A.V. Jones, M. Nelson.

Metal coordination compounds

Preparation and analysis of potassium tris(oxalato)ferrate(III) trihydrate [1984, **61**, 1098], J. Olmstead III.

The study of a cobalt complex—a laboratory project [1982, **59**, 1048], J.W. Loehlin, S.B. Kahl, J.A. Darlington.

Pedagogy

Popper's epistemology as a pedagogic and didactic principle, or: Let them make more 'mistakes' [1981, **58**, 565], W. Derkse.

A simple, safe and inexpensive laboratory exercise in the guided inquiry format [1987, **64,** 452], J.M. De Moura, Joseph A. Marcello.

Lab is a puzzle, not an illustration [1985, **62,** 874], M. Pickering.

Selected papers in chemical education research—implications for the teaching of chemistry

(Reproduced with permission of *International Journal of Science Education.*)

R.B. Bucat, P.J. Fensham, (191 pages) Price:USD5

Excerpts from preface

'Twenty research papers have been reproduced exactly as they appear in the journals in which they were published. These papers address six issues in chemistry teaching, and the monograph accordingly has six chapters…'

'On what grounds does a good teacher make decisions about how to teach chemical equilibrium, for example? The answer to this question is complex and wide-ranging, but part of the answer has to do with the teacher's pedagogical understanding of the subject matter. Most importantly, it involves seeing chemical equilibrium from the mind-set of the student. It involves recognising the particular difficulties that learning about chemical equilibrium presents. It involves understanding the characteristics of the ways of knowing (see Chapter 1) what are important for a rich understanding of chemical equilibrium, and how these are different from the important ways of knowing about oxidation-reduction, the chemistry of the alkenes, or stereochemistry, for example. It involves anticipating students' questions. It involves having a wide repertoire of teaching strategies, anecdotes, analogies and demonstrations that can be called upon when the occasion demands. It involves knowing what strategies do not 'work'. It involves being able to relate the subject matter to what the students already know and believe. It involves being able to plot a pathway that is challenging, that balances intellectual interest and cognitive demand, and that is good chemistry. Collectively, all of the above are sometimes called pedagogical content knowledge.

The first two chapters (1. What does it mean to 'know' chemistry? and 2. Teaching and learning) have been chosen for their general applicability to understanding the pedagogical content of any chemistry topic. The remaining four chapters, each related to a particular topic in chemistry, have been selected because they concern fundamental ideas on which much of the rest of chemistry depends. Research papers on the teaching and learning of other topics could constitute further volumes in a series of which this is the first.'

'We hope that this publication will at least arouse in its readers a consciousness that particular topics in chemistry need particular teaching and learning 'treatments'. Perhaps it will inspire the use of new strategies—which might follow the development of keener pedagogical content knowledge of at least those topics on which this monograph focuses. We believe that teachers can acquire pedagogical content knowledge in chemistry and the research in chemical education already has much to offer in this respect. Perhaps also this monograph might encourage some teachers to engage in research studies—no matter how small—in their own classroom, either in collaboration with teacher colleagues, or in partnerships with researchers from universities and colleges.'

'This publication must be regarded as an experiment. We had no precedent upon which to evaluate its approach or its utility. We invite chemistry teachers at any level to provide us with feedback and perhaps to relate ways in which it has influenced their teaching. If the reactions are sufficiently positive, perhaps the IUPAC Committee on Teaching of Chemistry may decide to publish more issue and so create a series.'

Chapter 1: What does it mean to 'know' chemistry?

Chapter 2: Teaching and learning

Chapter 3: Teaching and learning about chemical change

Chapter 4: Teaching and learning about the particulate nature of matter

Chapter 5: Teaching and learning about stoichiometry

Chapter 6: Teaching and learning about chemical equilibrium

Experiments with Low-Cost Equipment. K.V. Sané (Expected publication date: October 1995, Estimated Price: USD20).

This is a collection of about 100 experiments in both pure and applied chemistry which have been standardised by teachers all over the world using the low-cost equipment developed under the CTC/UNESCO Project.

Teaching of Environmental Chemistry. K.V. Sane (Expected publication date: October 1995, Estimated Price: USD20).

Section 1: Curriculum

This section will list and discuss the various curricula followed in different institutions all over the world. The objective of this section is to acquaint teachers and institutions with the current status of the teaching of Environmental Chemistry thereby enabling them to alter the scope and the content of their own curriculum. At the same time, it will provide a starting point to such institutions as do not have any courses in Environmental Chemistry but wish to formulate such courses.

Section 2: Teaching strategies

The objective of this section is to offer detailed information about some strategies for teaching of environmental chemistry. The emphasis will be on simple, modern and cost-effective techniques. This section should be of considerable relevance to teachers in developing countries who face a serious shortage of resources and therefore tend to neglect the laboratory part. The topics proposed to be included are:

(a) Low-cost equipment

(b) Small-scale chemistry

(c) Computer interfacing and simulation

(d) Audio-video based approaches

(e) Microprocessor-based do-it-yourself instrumentation

Section 3: Case studies and low-cost experiments

This section will include some case studies and several tested experiments developed by international and national agencies.

Environmental Chemistry Through Experiments—A Practical Approach. H.J. Bader, R. Blume, (1995, Estimated Price: USD10).

This is the English translation of the book *Umweltchemie I'm Experiment*, R. Blume, H.J. Bader (1989) Cornelsen Verlag Scriptor GmbH & Co., Frankfurt, Germany.

Classes in Coordination Chemistry. G.B. Kauffman (1995, Estimated Price: USD10).

This is a CTC Edition of *Classics in Coordination Chemistry* Part I, II and III translated, edited and with commentary by Prof George B. Kauffman, and Foreword by Prof G. Wilkinson, FRS. Part I of the original Dover publication—printed in 1968—contained translations of the six major papers of Alfred Werner, while Part II—published in 1976—comprised papers by German, Swedish, Danish, English and French chemists covering the period 1798 to 1899. Part III, published in 1977, completed the trilogy and consisted of ten papers by German, Russian, English and American scientists covering 20th century coordination chemistry from 1904 to 1935.

These books are published for IUPAC CTC by Shatabdi Computers Pvt. Ltd., Delhi 110 007 (India). Printed in India by Printing Production Service Centre, Delhi 110 009. CTC publications can also be ordered from Mr. P.J. Towse, Editor, INCE. C.S.S.M.E. University of Leeds, Leeds LS2 9JT, UK (Fax: +44 1132 334 683).

PAC Review

The June 1995, **67**(6), issue of *Pure and Applied Chemistry* contains the texts of the main lectures (plenary and invited), including the Rossini Lecture, presented at the Thirteenth International Conference on Chemical Thermodynamics (ICCT) held at Clermont-Ferrand, France, 17–22 July, 1994. The 13th ICCT was held jointly with the 25th AFCAT Conference (*Association Francaise de Calorimétrie et d'Analyse Themique*) under the sponsorship of IUPAC through the Physical Chemistry Division and Commission I.2 on Thermodynamics.

Reliable thermodynamic data concerning properties of pure substances and mixtures as well as chemical reactions are of prime importance for all the sciences. They are the basis for theoretical advances as well as for the development of new materials and processes. The large number and the scope of the papers presented in Clermont-Ferrand demonstrated the unabated, rapid growth of chemical thermodynamics. The program consisted of 21 plenary and invited (including the Rossini Lecture), 204 oral and 224 poster presenta-

tions organized into 10 symposia devoted to experimental, theoretical and applied aspects of thermodynamics in the following areas: experimental thermodynamics; nonelectrolyte mixtures/molecular fluids; aqueous solutions at superambient conditions; interfaces/polydispersed systems/colloids; biothermodynamics/health/environment; advanced materials and new technologies; polymeric materials; nuclear materials; fluid phase/energy/industrial; databases/databanks.

Four hundred and fifty scientists from 45 countries registered and the abstracts of 449 presentations have been collected in the conference programme book.

The *tenth Rossini Lecture* was presented by Hendrick C. Van Ness, Institute Professor Emeritus of Chemical Engineering at the Rensselaer Polytechnic Institute in Troy, New York, USA. His lecture was entitled *Thermodynamics in the treatment of vapour/liquid equilibria (VLE)data*.

Other notable scientific contributions presented at this conference included:

Hydrophobic hydration of small apolar molecules and extended surfaces: A molecular model *[a]N.A.M. Besseling and [b]J. Lyklema ([a]Akzo Nobel Central Research, PO Box 9300, Arnhem, the Netherlands, and [b]Physical and Colloid Chemistry, Wageningen Agricultural University, PO Box 8038, Wageningen, the Netherlands).*

The thermodynamic behaviour of water is special as compared to most other liquids. Its density passes a maximum with varying temperature at constant pressure, whereas for other fluids, and also for solids, the isobaric density is a monotonously decreasing function of temperature. The isothermal compressibility passes a minimum with varying temperature. Ice contracts upon melting into liquid water. Water has a large heat capacity and a high melting and boiling point as compared to other compounds of similar molecular mass. The surface tension, γ, of water is relatively high and surface entropy, $-d\gamma/dT$, passes through a maximum with varying temperature, whereas for simple fluids, such as argon, both γ and $-d\gamma/dT$ are monotonously decreasing functions.

One of the most intriguing properties of water, especially with regard to its role in biological systems, is referred to as the *hydrophobic effect*. This term is used to denote the anomalous behaviour of water as it interacts with apolar material. This is relevant, not only for the behaviour of simple aqueous solutions, but e.g. also for the conformation of proteins, the formation of micelles and biological membranes and for adsorption of surfactants at interfaces. The solubility of apolar compounds in water is low and passes a minimum at about room temperature upon varying temperature. This implies that the roles of entropy and enthalpy are unusual as compared to other mixtures. The precise value of the temperature of minimum solubility is somewhat different for each apolar compound.

These authors have modelled the hydrophobic hydration of small apolar molecules and of extended hydrophobic surfaces applying a statistical thermodynamical lattice–gas model. This model, in which the orientation-dependent interactions between water molecules (e.g. hydrogen bonds) are accounted for, reproduces the anomalous thermodynarnic behaviour of water. Moreover, in this model these macroscopic phenomena can be related to underlying molecular behaviour. The temperature dependencies of the density of pure water and of the solubility of small apolar molecules in water share a common molecular basis. Dissolution of small apolar molecules leads to a relatively small enhancement of the pronounced structuring that is intrinsically present in water. Formation of special 'iceberg-like' structures around apolar solutes does not occur. The negative solvation entropy is related to changes of the local ordering of the water molecules similar to those occurring upon expansion of pure water. Hydrogen bonding hardly decreases for these cases. The small, and at lower temperatures even negative, value of the solvation enthalpy is due to a reduction of the number of repulsive water-water interactions. Calculations on an extended flat hydrophobic surface indicate that the anomalous aspects of the solvation thermodynamics do not occur with bulky apolar particles. With these, a decrease of hydrogen bonding cannot be avoided and water tends to be depleted from such surfaces.

The balance between orientation-dependent attractive (hydrogen bonds) and repulsive interactions (nonhydrogen bonding contacts) leads to the open, approximately four-coordinated structure of water at ambient conditions, to the anomalous temperature dependencies of the isobaric density and of the solubility of apolar molecules (as well as to other properties that are not discussed here). The energy and entropy changes upon dissolution of small apolar molecules are related to changes of the distribution of intermolecular contacts. The molecular mechanism underlying the maximum of isobaric density of pure water is the same as for the minimum of the solubility of small apolar molecules as a function of temperature. The authors reject the idea that a region of specially structured water is present around a dissolved small apolar molecule. With regard to the structural changes incurred, the introduction of a small apolar solute is not very different from adding another vacancy. Upon adding a small apolar molecule in water, the number of hydrogen bonds decreases slightly, but the possibilities for realisation of these hydrogen bonds decreases strongly. Hence the entropy decrease. The low, for low temperatures, even negative value of the enthalpy change is due to a reduction of repulsive nonhydrogen bonding interactions

between water molecules. These changes are merely an enhancement of the kind of structuring that is intrinsically present in water. Similar changes occur upon expansion of pure water.

As an additional argument, they note that there is a certain analogy between the swelling of polymer networks and expansion of water. Upon swelling, by uptake of solvent, the entropy of a polymer network decreases. This is easily explained: since the bonds in a polymer network do not break, the configurational freedom of the polymer segments decreases upon expansion of the network and hence the entropy. Upon expansion of pure liquid water, or by uptake of small apolar molecules, the number of hydrogen bonds between water molecules does not decrease much and consequently the configurational freedom of the water molecules decreases. Water can in some respects be considered as a network of molecules connected by hydrogen bonds. However, the lifetime of a hydrogen bond is short and the hydrogen bonds are reshuffling all the time. This mechanism will hold for small solutes of similar size as the water molecules and for slender apolar chains. It will break down for bulky solutes and for the hydration of extended surfaces. The latter will inevitably lead to *qualitative* changes of adjacent water as compared to the bulk, and to more substantial reduction of the number of hydrogen bonds. According to the author's calculations, both the thermodynamics and the changes of water structure differ qualitatively from the case of small apolar molecules. Adjacent to the apolar surface water is depleted. The resulting temperature dependencies of the enthalpy and entropy of solvation do not exhibit the behaviours typical for the 'hydrophobic effect'.

Dissolution and crystallization rates of silicate minerals as a function of chemical affinity. *J. Schott and E. H. Oelkers (Laboratoire de Geochimie, CNRS/Universite Paul-Sabatier, Toulouse, France).*

Detailed knowledge of silicate dissolution/precipitation kinetics at conditions characteristic of geochemical processes is essential to understanding the rate and extent of chemical mass transfer and water/rock interaction both in and on the surface of the Earth. With the exception of some Earth surface systems, for example, environmental pollution and chemical weathering, these processes occur at near to equilibrium conditions. Thus, there is a strong need for kinetic rate equations that allow the extrapolation of mineral dissolution and crystallization rates measured in the laboratory at far from equilibrium conditions to the near to equilibrium conditions typical of natural processes.

Prior to 1992, the variation of silicate dissolution/crystallization rates with chemical affinity was generally believed to follow a behaviour consistent with transition state theory (TST), and the assumption that (i) a single elementary reaction dominates the dissolution rates at all affinities, and (ii) the activated or precursor complex controlling this hydrolysis has the same Al/Si ratio as the reacting mineral. According to these assumptions, the constant pH reaction rates are independent of solution saturation state at far from equilibrium conditions, and a simple function of chemical affinity at near to equilibrium conditions. Recent experimental investigations of silicate dissolution as a function of solution saturation state permit the testing of rate laws derived from TST with the above assumptions. Of the minerals thus far investigated, quartz and anorthite were found to obey this rate equation, but albite, potassium-feldspar, kyanite and kaolinite dissolution rates were found to exhibit different behaviours. These results imply that the rate-limiting reaction step is not the same for all silicates and depends on the individual mineral structure.

The variation of silicate dissolution and crystallization rates with chemical affinity and solution composition can be quantified by the identification of the rate controlling precursor complex. The nature of this complex depends on the individual mineral structure. Specifically, the destruction of quartz and anorthite frameworks requires the breaking of only one type of structural group. For these minerals, the rate controlling precursor complex has the composition of the mineral itself plus or minus H^+, OH^- and/or H_20. As a result, the hydrolysis rates of these minerals do not depend on either the aqueous Al/Si ratio or chemical affinity far from equilibrium conditions. In contrast, the destruction of the kaolinite, albite, potassium feldspar, and kyanite frameworks requires the breaking of more than one structural group. For these minerals the rate controlling precursor complex has a different Al/Si ratio from the mineral and their hydrolysis rates have been found to depend on the aqueous Al/Si ratio. These rates thus appear to depend on chemical affinity far from equilibrium conditions. Taking into account the identity of these precursor complexes and the framework of transition state theory leads to equations that can accurately describe the hydrolysis rates of each of these minerals as functions of pH, aqueous aluminium and silica concentration, and chemical affinity.

Within the framework of transition state theory, the rate of an elementary reaction is proportional to the concentration of the activated complex (or free energy maximum that the reactants should pass to be converted into products). Wieland *et al.* demonstrated that the rate is also proportional to the concentration of the surface species precursor of the activated complex (precursor complex). Although silicate dissolution likely involves several elementary reactions, TST can still be applied to the overall rate if it is controlled by a single

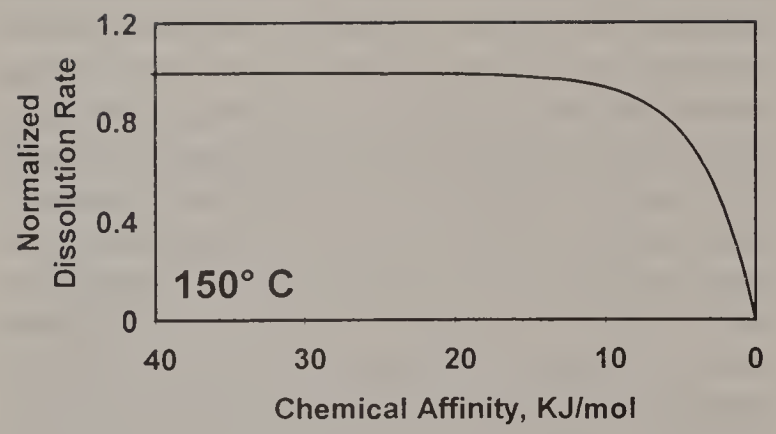

Fig. 1 Variation of mineral dissolution rate with chemical affinity as predicted by eqn (2).

elementary rate-limiting step. Within this context, silicate dissolution rates can be described using

$$r = k_+ \mathrm{P}a_i^{-n}{}_i \{ 1 - \exp(-A/\mathrm{s}RT)\}, \quad (1)$$

where r defines the net reaction rate, k_+ denotes a dissolution rate constant, a_i corresponds to the activity of the ith aqueous species, n_i signifies the reaction coefficient of the ith species in the reaction forming the precursor complex, s refers to the reaction order, A denotes the chemical affinity for the overall reaction, T stands for absolute temperature, and R represents the gas constant.

The product $\Pi a_i^{-n}{}_i$ describes the effect on the overall rate of the activities of the aqueous species involved in precursor complex formation. The terms within the brackets describe the effect of solution saturation state. For highly undersaturated solutions, A has a large positive value and the term within the brackets is equal to 1. At these conditions the dissolution rate is independent of chemical affinity (or bulk solution saturation index), but is still dependent on the activities of the aqueous species that participate in the formation of the precursor complex. For small deviations from equilibrium (i.e. when $A/\sigma < RT$), the rate becomes linearly related to chemical affinity.

When applying eqn (1) to silicate dissolution rates, it is commonly assumed that (i) H^+, OH^- and H_2O are the only aqueous species involved in precursor complex formation, (ii) a single reaction mechanism controls the overall rate at all chemical affinities, and (iii) $\sigma \sim 1$. These assumptions lead to the following rate equation

$$r = k\phi_+ (a_{H+})^{nH+} \{ 1 - \exp(-A/RT)\}, \quad (2)$$

where $k\phi_+$ refers to the dissolution rate constant for the hydrolytic process. This rate law has been used extensively to model water–rock interactions in the crust. The adoption of eqn (2) leads to predictions of mineral dissolution/crystallisation rates as a function of chemical affinity at constant pH as illustrated in Fig. 1. It can be seen in this figure that eqn (2) implies that silicate dissolution rates are independent of chemical affinity at far from equilibrium conditions (i.e. $A > 10$ kJ/mol at 150 °C) and decrease with A at close to equilibrium conditions.

The results presented here demonstrate that the hydrolysis of mixed oxide silicates is a multi-step process involving the breaking of several different bonds (see Fig. 2). Thus the rate laws controlling these reactions depend on the structure and chemistry of the mineral's near-surface region. The key to the hydrolysis of most aluminosilicates is the destruction of the oxide polymer composed of silicate and aluminate groups. As aluminate groups are much more reactive than silicate groups, the Al/Si ratio exerts an important control on the mechanism of polymer framework destruction. When the Al/Si ratio is small, as in alkali feldspars, aluminate sites can be completely removed without dramatically increasing the porosity of the solid and the rate limiting

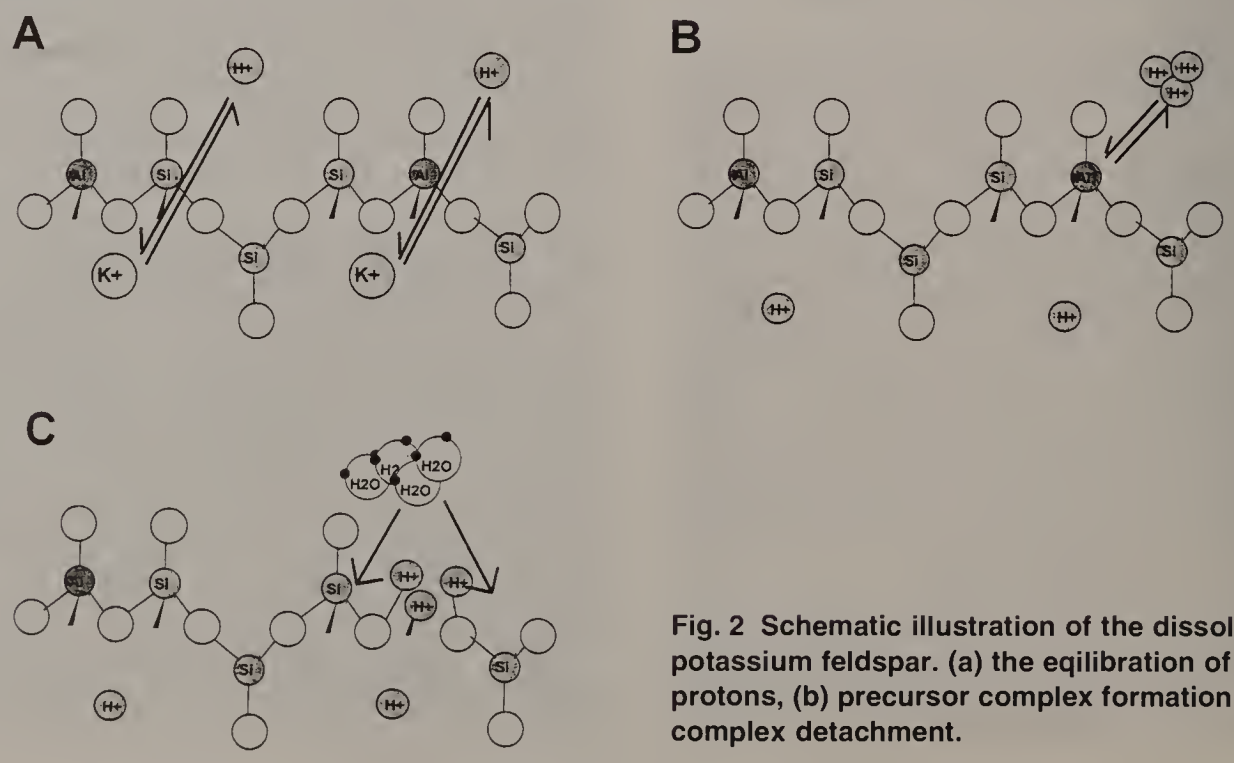

Fig. 2 Schematic illustration of the dissolution of potassium feldspar. (a) the eqilibration of alkali with protons, (b) precursor complex formation, (c) precursor complex detachment.

step for dissolution, as for quartz, is the breaking of Si–O bonds. At the other structural extreme, in minerals like olivines exhibiting a crosslink density of zero, the hydrolysis of modifier cation–oxygen bonds is likely rate limiting, permitting isolated silicate units to be directly converted to aqueous silica.

It is possible from structural considerations, surface chemistry determinations and measurements of reaction rates as a function of chemical affinity and solution composition, to characterise the rate limiting step and the precursor complex stoichiometry of several aluminosilicates. Taking account of precursor complex forming reactions and TST leads to equations than can accurately describe the variation of these rates with respect to solution composition and chemical affinity. The stoichiometry of these rate controlling Si-rich, Al-deficient precursor complexes has two important applications for geochemical processes: (i) in agreement with observations made on natural hydrothermal and sedimentary systems, the dissolution/crystallization rates predicted by this revised interpretation are up to several orders of magnitude lower than previously postulated and, (ii) crystallization rate constants of many aluminosilicate minerals may be similar to that of quartz.

Recent Reports

In this section we publish summaries of the most recent IUPAC recommendations on nomenclature and symbols and technical reports. The full texts of these recommendations and reports are published in *Pure and Applied Chemistry.*

Critical evaluation of the stability constants of metal complexes of amino acids with polar side chains (Technical report)

Available experimental data on proton and metal complex equilibria of the seven essential amino acids with polar side chains (i.e. cysteine, cystine, methionine, serine, threonine, asparagine and glutamine) have been critically evaluated. First, the introduction outlines the main structural features of these amino acids as ligands and calls attention to their important roles in biology. A general discussion is also reported on the determination of formation constants and their reliability. In particular, the critical role played by protonation constants as reference parameters for the determination of complex formation constants by glass electrode potentiometry has been emphasized. Coordination enthalpies and entropies are also introduced, and the selection criteria employed in the course of the review are described.

For each of the seven amino acids, a specific chapter then reports (i) protonation constants and their associated enthalpic and entropic changes, (ii) formation constants for binary metal complex species and ternary mixed-ligand complexes with the associated thermodynamic quantities whenever available. For each entry, all the data available in the literature are first reported. Then, a selection of recommended or tentative values is proposed for as many sets of specific experimental conditions as possible, in accordance with the criteria given in the introduction and based on considerations developed in corresponding discussions.

This report was prepared by G. Berthon (INSERM U305, Equipe 'Bioréactifs: Spéciation et Biodisponibilité', 38 rue des Trente-six Ponts, Toulouse 31400, France) for the Commission on Equilibrium Data of the Analytical Chemistry Division. The full details are to be found in Pure Appl. Chem. 1995, ***67****(7), 1117–1240.*

Microbial production of commodity chemicals (Technical report)

Microbial processes for industrial production of commodity chemicals are rapidly gaining practical significance for preparation of high purity products, in an environmentally acceptable manner while realizing energy savings. The use of bacterial nitrile hydratase for industrial production of the important chemical, acrylamide, was recently pioneered in Japan. We review here the enzymatic production of acrylamide and recent progress in the production of other commodity chemicals through microbial processes.

This report was prepared by by T. Nagasawa and H. Yamada (*Department of Biological Function & Genetic Resources Science, Okayama University, 1-1-1 Tsushima Naka, Okayama 700, Japan and Toyama Prefectural University, Kurokawa, Kosugi, Imizu-gun, Toyama 939, Japan) for the Commission on Biotechnology of the Applied Chemistry Division (now*

*called the Division of Chemistry and the Environment). The full details are to be found in Pure Appl. Chem. 1995, **67**(7), 1241–1256.*

Manual of methods and procedures for catalyst characterization (Technical Report)

The manual provides details and recommendations concerning the experimental methods used in catalysis. The objective is to provide recommendations on methodology (rational approaches to preparation and measurements). It is not intended to provide specific methods of preparation or measurement, nor is it concerned with terminology, nomenclature, or standardization.

*This report was prepared for publication by J. Haber[1], J. H. Block[2] and B. Delmon[3] ([1]Polish Academy of Sciences, Research Labs. of Catalysis & Surface Chemistry, ul. Niezapominajek, PL-30 239 Krakow, Poland, [2] Fritz-Haber Institute der Max-Planck Gesellschaft, Faradayweg 4-6, D-1000 Berlin 33/Dahlem, Germany, and [3] Unité de Catalyse et Chimie des Matériaux Divisés (CATA), Place Croix du Sud 2/17,Université Catholique de Louvain, B-1348 Louvain-la-Neuve, Belgium). For the Subcommittee on Catalyst Characterization of the Commission on Colloid and Surface Chemistry of the Physical Chemistry Division. The full details are to be found in Pure Appl. Chem. 1995, **67**, 1257–1306.*

Glossary of class names of organic compounds and reactive intermediates based on structure (IUPAC Recommendations 1995)

This is a glossary of terms used to denote classes of compounds, substituent groups and reactive intermediates, in contrast to individual compounds. The overwhelming majority of the terms refer to organic compounds, but a few classes that may be considered inorganic are included for convenience. The principal criterion for inclusion is that the class be definable by structure.

*This report was prepared for publication by G.P. Moss, P.A.S. Smith and D. Tavernier. For the Organic Chemistry Division. The full details are to be found in Pure Appl. Chem. 1995, **67**, 1307–1375.*

Units for use in atmospheric chemistry (IUPAC Recommendations 1995)

This document examines the utility and suitability of the International System of Units (Système International, SI) as a framework for units in atmospheric chemistry and presents recommendations regarding use of these units in reporting atmospheric chemistry data consistent with the special requirements of this subdiscipline.

Table 1 Symbols, SI units and common units for quantities in atmospheric chemistry (Taken from the report prepared by S. E. Schwartz and P. Warneck. The details are to be foumd in *Pure Appl. Chem.* 1995, 67, 1377–1406).

Quantity	Symbol	Si Unit	Common Unit
altitude	z	m	m, km
radius of aerosol particles and cloud drops	r, a	m	μm, mm
wavelength (of light)	λ	m	nm, μm
area	A	m^2	m^2, km^2, μm^2 ...
volume	V	m^3	m^3, dm^3, μm^3 ...
deposition velocity	v_d	$m\ s^{-1}$	$cm\ s^{-1}$
pressure	p	Pa	hPa, kPa, MPa
mass content of a substance s in an atmospheric region	G_S	kg	Tg, Pg
tropospheric mass	G_T	kg	kg, Zg
mass column density (of substance s)	W_S	$kg\ m^{-2}$	$kg\ m^{-2}$
mass density of air	ρ_{air}	$kg\ m^{-3}$	$kg\ m^{-3}$
mass density of water	ρ_w	$kg\ m^{-3}$	$kg\ m^{-3}$, $g\ cm^{-3}$
chemical amount concentration of a substance s in air	c_S, $c_a(s)$	$mol\ m^{-3}$	$mol\ m^{-3}$
number concentration of a substance s in air	n_S, C_S, $c_n(s)$	m^{-3}	$molecule\ m^{-3}$ $molecule\ cm^{-3}$
mass concentration of a substance s in air	c_S, $c_m(s)$	$kg\ m^{-3}$	$kg\ m^{-3}$, $g\ m^{-3}$, ...
chemical amount concentration of a substance s in aqueous solution	[s]	$mol\ m^{-3}$	$mol\ m^{-3}$, $mol\ dm^{-3}$
molality of a substance s in aqueous solution	m_S, $m(s)$	$mol\ kg^{-1}$	$mmol\ kg^{-1}$, $\mu mol\ kg^{-1}$, ...
mole fraction of a substance s in air	x_S, $x(s)$	1	$mol\ mol^{-1}$, $\mu mol\ mol^{-1}$, ...
mass mixing ratio of a substance s in air	w_S	1	$kg\ kg^{-1}$, $g\ kg^{-1}$, ...
liquid water mass concentration in air	L	$kg\ m^{-3}$	$kg\ m^{-3}$, $g\ m^{-3}$, ...
chemical reaction rate	r	$mol\ m^{-3}\ s^{-1}$	$mol\ m^{-3}\ s^{-1}$, $molecule\ m^{-3}\ s^{-1}$ $molecule\ cm^{-3}\ s^{-1}$
unimolecular reaction rate coefficient	k_{uni}	s^{-1}	s^{-1}

In general, SI is well suited for application to atmospheric chemistry; specifically the wide range of magnitudes that are encountered can be dealt with by the prefixes denoting multiples and submultiples of units, and the application of SI units leads automatically to consistency in unit calculus. The use of special names and symbols for units that are not part of the SI, and are not products of powers of SI base units is discouraged; examples are: atmosphere, Dobson unit, hectare. However, continued use of such units (especially the Dobson unit) alongside SI units is advisable for a time until the SI units become more familiar. Local abundances of substances in air may be expressed as mixing ratios or concentrations. Mixing ratio has the advantage of being independent of pressure or temperature, but concentration has advantages for reaction kinetics and material transport. Amount-based units for mixing ratios or concentrations of substances of known chemical composition are preferable to mass-based units. The dimensionless unit mol per mol of air is recommended for mixing ratio of a substance in air, e.g. nmol/mol, rather than the customary parts per billion (ppb). It is necessary to specify whether a mixing ratio refers to dry or moist air. Expressing mixing ratios as 'reduced concentrations' relative to standard conditions of pressure and temperature leads to ambiguity and should be avoided where possible. Gas-phase concentrations may be expressed on the basis of either mole (mol m^{-3}) or molecule (molecule m^{-3}; SI: m^{-3}). The universal use of a single set of units for gas-phase concentration does not seem forthcoming in the immediate future, although the use of mol m^{-3} affords advantages of consistency and convenience. An extensive table of recommended symbols and SI units for quantities in atmospheric chemistry is presented.

Table 1 Continued

quantity	symbol	Si Unit	Common Unit
bimolecular reaction rate coefficient	k_{bim}	m^3 mol^{-1} s^{-1}	m^3 mol^{-1} s^{-1} m^3 $molecule^{-1}$ s^{-1} cm^3 $molecule^{-1}$ s^{-1}
termolecular reaction rate coefficient	k_{ter}	m^6 mol^{-2} s^{-1}	m^6 mol^{-2} s^{-1} m^6 $molecule^{-2}$ s^{-1} cm^6 $molecule^{-2}$ s^{-1}
chemical amount flux for substance s	$F_a(s)$	mol m^{-2} s^{-1}	mol m^{-2} s^{-1}
number flux for substance s	$F_n(s)$	m^{-2} s^{-1}	molecule m^{-2} s^{-1}
mass flux for substance s	$F_m(s)$	kg m^{-2} s^{-1}	kg m^{-2} s^{-1}
radiant energy flux	J	W m^{-2}	W m^{-2}
photon number flux	I_n	m^{-2} s^{-1}	photon m^{-2} s^{-1}
photon amount flux	I_a	mol m^{-2} s^{-1}	mol m^{-2} s^{-1}
molecular absorption cross section	σ	m^2	m^2 $molecule^{-1}$, cm^2 $molecule^{-1}$
molar Naperian absorption coefficient	κ	m^2 mol^{-1}	m^2 mol^{-1}
photodissociation coefficient	j	s^{-1}	s^{-1}
quantum yield	ϕ	1	molecule $photon^{-1}$
molecular diffusion coefficient	D	m^2 s^{-1}	m^2 s^{-1}
eddy diffusion coefficient	K	m^2 s^{-1}	m^2 s^{-1}
local production rate for substance s	$q_a(s)$	mol m^{-3} s^{-1}	mol m^{-3} s^{-1}
	$q_n(s)$	m^{-3} s^{-1}	molecule m^{-3} s^{-1}
	$q_m(s)$	kg m^{-3} s^{-1}	kg m^{-3} s^{-1}
local sink rate for substance s	$s_a(s)$	mol m^{-3} s^{-1}	mol m^{-3} s^{-1}
	$s_n(s)$	m^{-3} s^{-1}	molecule m^{-3} s^{-1}
	$s_m(s)$	kg m^{-3} s^{-1}	kg m^{-3} s^{-1}
integrated source strength for substance s	$Q_a(s)$	mol s^{-1}	mol a^{-1}
	$Q_n(s)$	s^{-1}	molecule a^{-1}
	$Q_m(s)$	kg s^{-1}	kg a^{-1}
integrated sink strength for substance s	$S_a(s)$	mol s^{-1}	mol a^{-1}
	$S_n(s)$	s^{-1}	molecule a^{-1}
	$S_m(s)$	kg s^{-1}	kg a^{-1}

*This report was prepared for publication by S. E. Schwartz[1] and P. Warneck[2] ([1]Environmental Chemistry Division, Brookhaven National Laboratory, Upton, NY 11973, USA, and [2]Abteilung Biogeochemie, Max-Planck-Institut fur Chemie, Saarstr. 23, D-55020 Mainz, Germany). For the Commission on Atmospheric Chemistry of the Applied Chemistry Division. The full details are to be found in Pure Appl. Chem. 1995, **67**, 1377–1406.*

Local air pollution in fast developing countries (Technical Report)

Local air pollution is one of the most pressing environmental problems in developing countries. The patterns of local air pollution are similar in many countries. In the initial stages of economic development the demand for energy, coupled to economic expansion, rises sharply. This increased consumption of power for heating, electricity, industrial processes etc. must lead to an increase of emissions. Dust, SO_2 and secondary products like sulfuric acid are responsible for severe impairments of human health and large scale damage to nature and buildings. Many developing countries have reached this stage of local air pollution or will

be exposed to this type of environmental hazards in the near future. Economically developed countries, like the US, Japan and many countries in Western Europe have passed this stage one to three decades ago. In the next phase of economic development transportation, especially by means of lorries and cars becomes a determining factor in local air pollution and cause high concentrations of ozone, peroxyacetyl nitrate (PAN) and other oxidants are present as secondary products of traffic emissions. A number of developing countries are now entering the stage when this 'Los Angeles' type of smog starts to become an important environmental problem. Developing countries should benefit from transfer of knowledge obtained in research programs and development of abatement policies m countries, which have been exposed to these problems in the past. But exchange of ideas between developing countries, regarding assessment of air pollution and implementation of emission controls is also very useful to derive optimal abatement strategies.

Report based on Proceedings of the International Workshop held in Cheng De, near Beijing (China), 20–21 July 1994. Organized by the Center for Environmental Sciences, Peking University, Beijing, in collaboration with the Netherlands Energy Research Foundation (ECN) and the Council for Environmental Relations, China/Netherlands

*This report was prepared for publication by J. Slanina[1], R. H. Brown[2] and X. Tang[3] ([1]Stichting Energieonderzoek Centrum Nederland, PO Box 1, 1755 ZG Petten, Netherlands, [2]Health & Safety Laboratory, Health & Safety Executive, Broad Lane, Sheffield S3 7HQ, UK, and [3]Center of Environmental Sciences, Peking University, Beijing, China). For the Commission on Atmospheric Chemistry of the Applied Chemistry Division. The full details are to be found in Pure Appl. Chem. 1995, **67**, 1407–1486.*

Detection and significance of active metabolites of agrochemicals and related xenobiotics in animals (Technical Report)

The production of active metabolites from agrochemicals, particularly pesticides, is a common event and often determines the nature and extent of the toxicological responses observed in both target and non-target species. The various pathways of mammalian metabolism by which agrochemicals are converted to toxicologically more active metabolites are reviewed and illustrated with examples. Methods to detect, measure and study active metabolites are discussed. The relative importance of these pathways are compared in various test animals and humans and other factors influencing the pathways of production and destruction of active metabolites are described. It is concluded that improved approaches to risk assessment are needed for agrochemicals that, where appropriate, take into account the complexities of their activation reactions and of species differences in the generation and responses to active metabolites.

*This report was prepared for publication by R. M. Hollingworth[1], N. Kurihara[2], J. Miyamoto[3], S. Otto[4] AND G. D. Paulson[5] ([1]Pesticide Research Center, Michigan State University, E. Lansing, MI 48824, USA, [2]Radioisotope Research Center, Kyoto University, Kyoto 606, Japan, [3]Sumitomo Chemical Co. Ltd., Kitahama 4-Chome 5-33, Chuo-Ku, Osaka 451, Japan, [4]BASF, Landwirtschaftliche Versuchsstation, D(W)-6703, Limburgerhof, Germany, and [5]USDA-ARS, Biosciences Research Laboratory, Fargo, ND 58105, USA). For the Commission on Agrochemicals of the Applied Chemistry Division. The full details are to be found in Pure Appl. Chem. 1995, **67**, 1487–1532.*

Use of immunoassays for the analysis of pesticides and some other organics in water samples (Technical Report)

Immunoassay (IA) kits were first developed for use in the medical field where they now have extensive usage, but over recent years many kits have been developed for determining pesticides and other organic chemicals in environmental samples. This paper provides a draft specification for EIA kits and an experimental design for validation of their performance. Enzyme immunoassay (EIA) kits available commercially for analysis of organic chemicals in water are reviewed in the light of the proposed requirements for analysis of pesticides in drinking water. Finally, some recommendations are given regarding the use of the kits under laboratory and field conditions.

*This report was prepared for publication by C. D. Watts and B. Hegarty (WRc plc, Medmenham Laboratory, Henley Road, Medmenham, Marlow, Bucks, SL7 2HD, UK). For the Commission on Water Chemistry of the Applied Chemistry Division. The full details are to be found in Pure Appl. Chem. 1995, **67**, 1533–1548.*

In-situ and on-site treatment of groundwater (Technical Report)

This paper reviews the possibilities of in-situ and on-site treatment of groundwater as a feasible alternative method for remediation of subsurface petroleum and other chlorinated hydrocarbons to 'Pump and Treat' followed by recharge to the aquifer or offsite disposal. In-situ bioremediation has however its limita-

tions. Not all the contaminants are biodegraded or eliminated. High microbial growth rates can occur in the near-field of the injection well, reducing permeability and well capacity. The efficiency also depends on local hydrogeological conditions and is limited to areas at which hydrogeological data are well established. Lack of reliable information on application, performance and cost are also a major impediment to its use. Recent estimates for the Superfund Program, indicate that the average cost is about $1.7m per site, very close to the present estimate of $2.5m for the cleaning of about 400 cu.m of jet fuel from a contaminated site in Israel. These estimates are significantly lower as compared to the average cost of $12.5m for a pump and treat system. The total sums are substantial and are indicative to a fast developing technology and a growing market for innovative clean-up processes. Concerted efforts are still required to develop techniques for cleaning of groundwater employing integrated research approach, combining biotechnology with environmental engineering. However, the prospects for feasible combination of below and above ground processes, competitive costs, reduced residuals and positive environmental impacts as reported in this review give reason for optimism.

*This report was prepared for publication by Y. Shevah[1] and M. Waldman[2] ([1]Tahal Consulting Engineers Ltd., 54 Rehov IBN Gvirol, Tel-Aviv 61111, Israel, and [2]National Council for Research & Development, Ministry of Science and Technology, Bldg. 3, Eastern Secretariat, PO Box 18195, Jerusalem 91181, Israel). For the Commission on Water Chemistry of the Applied Chemistry Division. The full details are to be found in Pure Appl. Chem. 1995, **67**, 1549–1561.*

Properties and units in the clinical laboratory sciences—I. Syntax and semantic rules (IUPAC–IFCC Recommendations 1995)

This document is an updating of previous recommendations on the presentation of properties and their values in clinical laboratory sciences from IFCC, IUPAC and WHO.

It forms part of the ongoing effort towards 'standardization' of *transmission* of laboratory request and report across cultural/language domains while avoiding standardization of the language used by clinicians or laboratory practitioners.

Subsequent documents will list the kinds-of-property and the properties used in clinical laboratory sciences.

*This report was prepared for publication by H. Olesen (Dept. of Clinical Pharmacology Q 76.4.2, National University of Copenhagen (Rigshospitalet) Tagensvej 20, DK-2200 Copenhagen, Denmark). For the Commission on Quantities and Units in Clinical Chemistry of the Clinical Chemistry Division and for the International Federation of Clinical Chemistry. The full details are to be found in Pure Appl. Chem. 1995, **67**, 1563–1574.*

Sample collection guidelines for trace elements in blood and urine (Technical report)

This paper presents an organized system for element-specific sample collection and handling of human blood (whole blood, serum or plasma, packed cells or erythrocytes) and urine also indicating a proper definition of the subject and sample. Harmonized procedures for collection, preparation, analysis and quality control are suggested. The aim is to assist scientists worldwide to produce comparable data which will be useful on a regional, national and international scale. The guidelines are directed to the elements aluminium, arsenic, cadmium, chromium, cobalt, copper, lead, lithium, manganese, mercury, nickel, selenium and zinc. These include the most important elements measured for their occupational or clinical significance, and serve as examples of principles that will guide development of methods for other elements in the future.

*This report was prepared for publication by R. Cornelis[1], B. Heinzow[2], R. F. M. Herber[3], J. Molin Christensen[4], O. M. Paulsen[4], E. Sabbioni[5], D. M. Templeton[6], Y. Thomassen[7], M. Vahter[8] and O. Vesterberg[9] ([1]Laboratory of Analytical Chemistry, University of Gent, Proeftuinstraat 86, B-9000 Gent, Belgium, [2]Institute for Environmental Toxicology of Schleswig-Holstein, D-2300 Kiel, Germany, [3]Coronel Laboratory for Occupational & Environmental Health, University of Amsterdam, Netherlands, [4]National Institute for Occupational Health, DK-2100 Copenhagen O, Denrnark, [5]EC Research Centre, Environmental Toxicology Unit, CCR, I-21 020 Ispra, Varese, Italy, [6]Department of Clinical Biochemistry, University of Toronto, Toronto, Ontario M5G IL5, Canada, [7]National Institute of Occupational Health, PO Box 8149 Dep., N-0033 Oslo, Norway, [8]Karolinska Institute of Environmental Medicine, PO Box 210, S-17177 Stockholm, Sweden, and [9]National Institute of Occupational Health, S-171 84 Solna, Sweden). For the Working Party of the Commission on Toxicology of the Clinical Chemistry Division. The full details are to be found in Pure Appl. Chem. 1995, **67**, 1575–1608.*

IUPAC colleague deceased

Prof. R. P. Graham (24 June 1995)
Commission on Physicochemical Measurements and Standards (1959–1981)

Affiliate Affairs

Information for affiliates

IUPAC publications

Affiliates are entitled to a 25% reduction, and in some cases a 40% reduction on the cost of IUPAC publications except *Pure and Applied Chemistry*. A leaflet detailing IUPAC books currently available from Blackwell Science Ltd has recently been distributed by the publishers to all *CI* readers. Further copies may be obtained from the IUPAC Secretariat.

How to contact commissions

IUPAC affiliates may if they wish communicate directly on scientific matters with the officers of IUPAC commissions. A full list of names and addresses of all commission officers for 1996–97 was published in the November 1995 issue of *CI*.

Affiliate reduction of conference registration fees

It is a condition of IUPAC sponsorship of a conference that IUPAC affiliates are entitled to a 10% reduction or 'own members' rate on the registration fee for scientific participants. This concession is usually, but not always, announced in the conference circulars and indicated on the registration form.

To receive this reduction an affiliate must declare on the conference registration form that (s)he is an affiliate. Alternatively the affiliate should apply in writing to the conference organizer for this reduction stating that (s)he is an affiliate. Conference organizers may check with the IUPAC Secretariat that applicants for this reduction are currently registered as affiliates.

If an application for this reduction is refused, an affiliate should immediately notify the Affiliate Affairs Secretary and, if possible, forward copies of documentary evidence of this refusal.

Visas

It is a condition of sponsorship that organizers of meetings under the auspices of IUPAC, in considering the locations of such meetings, should take all possible steps to ensure the freedom of all bona fide chemists from throughout the world to attend irrespective of race, religion, or political philosophy.

IUPAC sponsorship implies that entry visas will be granted to all bona fide chemists provided application is made not less than three months in advance. If a visa is not granted one month before the meeting the IUPAC Secretariat should be notified without delay by the applicant.

Address of IUPAC Secretariat

Please use the following address for all communications directed to the IUPAC Affiliate Affairs Secretary. If your are submitting a letter for publication in *Chemistry International* (*CI*), please indicate that the letter is 'Submitted for publication in *CI*.'

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Cowley, Oxford OX4 3YF, UK.

Tel: +44 (1865) 747744
Fax: +44 (1865) 747510
E-mail: iupac@vax.oxford.ac.uk

Ties and scarves

Ties and scarves emblazoned with the IUPAC logo may be purchased from the IUPAC Secretariat by applying to the Affiliate Affairs Secretary. The colours for both are *either* maroon *or* dark blue. The ties cost USD 14.00/GBP 7.00 each and the scarves USD 12.00/GBP 6.00 (including postage and packing).

Please use the form (or a photocopy of it) published on page 24 of the January 1994 issue of *CI*. Alternatively please write to the Affiliate Affairs Secretary with your order stating the colour you require. A cheque made payable to IUPAC for the appropriate amount should be enclosed with your order.

IUPAC poster

Copies of an IUPAC poster are available **free of charge** to affiliates and members of IUPAC's commissions and committees. The poster is printed in maroon and black on a white background and is approximately 42 × 59 cm in size.

IUPAC welcomes any publicity you can give to its activities. If you would like to display one or more copies of the poster in your department or elsewhere please write to the Affiliate Affairs Secretary stating your name and address and how many copies of the poster you wish to receive.

IUPAC-sponsored conferences

An updated list of names and addresses of the organizers of all future IUPAC sponsored conferences is given in the 'Conference Calendar' published in each issue of *CI*.

The Affiliate Membership Programme: Input from readers of Chemistry International

As a reader of *Chemistry International (CI),* here is your chance to contribute to a 'new look' for the Affiliate Membership Programme.

At the meeting of Council, 38th IUPAC General Assembly, Guildford, UK, August, 1995, the Bureau proposed that the IUPAC Affiliate Membership Programme (AMP) be discontinued. The proposal arose from a report to the Bureau that the AMP was losing money, and that changes to its operation were needed which would guarantee no financial loss to IUPAC. After much discussion, the proposal was defeated decisively by Council; the final recommendation was that the AMP be continued at least until the 39th IUPAC General Assembly in Geneva in 1997.

Following the meeting of Council, the Bureau reconstituted the Committee on Affiliate Membership (CAM) to examine how the AMP could be modified to make it financially self-sufficient and more attractive to current and prospective members. The members of CAM are: Prof. A. Chakravorty (India), Dr. D. F. Eaton (USA) and Prof. J. W. Lorimer (Canada; Chairman), all elected members of the Bureau, together with Dr. J. H. Williams (Secretary).

As a first stage, CAM has circulated a questionnaire to the National Adhering Organizations and their National Committees for IUPAC for suggestions about the AMP. It was also decided to publish the questionnaire in *CI* so that all readers could have an opportunity to reply.

Unlike many questionnaires which leave space for replies, we want to encourage extensive written comments on all points. The questions follow.

A. Financial arrangements

The cost of becoming an Affiliate is essentially the price of six issues of *CI*, plus a secretarial overhead—there is a considerable amount of work done at the Oxford Secretariat for AMP. On top of this IUPAC component, (currently USD14.20 which will increase to USD16 from 1 January 1996) there is the amount charged by the National Chemical Society, which varies from country to country. Increases in the membership fee are due mainly to increases in costs of printing *CI*.

1. Do you consider the current fee for Affiliate Membership of IUPAC to be reasonable?

2. Would you support: (a) an immediate (but modest) additional increase in the membership fee to help make the programme more financially self-sufficient; (b) subsequent annual reviews to adjust for inflation?

3. For countries without a National Chemical Society, and even for some Member and Observer Countries of IUPAC, the annual membership fee, in US dollars, may be large enough to discourage participation by many chemists. One suggestion to alleviate this problem would be to establish the membership fee as a fixed percentage of the membership fee of the particular National Chemical Society. What do you think of this suggestion? Do you have other suggestions? (The committee has asked the National Chemical Societies for their fee structure to aid in evaluating replies to question 3.)

B. Membership

4. At present, contributors to IUPAC programmes need not be Affiliates of IUPAC. The number of contributors listed in the IUPAC Handbook who are also Affiliates is not known precisely, but is estimated to be significant. A show of hands at the last Council meeting indicated that most members of Council are, in fact, Affiliates. Do you feel that Affiliate Membership (or whatever name is given ultimately; see next question) should be a requirement for all contributors to IUPAC programmes?

5. The term Affiliate may have negative connotations for current and prospective members. Do you feel that a change from Affiliate to simply Member would make the programme more attractive?

6. It has been suggested that, to recognize past contributions and to encourage continued participation, former participants in IUPAC programmes be enrolled as IUPAC Fellows, provided that they pay the regular Affiliate Membership fee. Do you approve of this idea?

C. Benefits to Affiliate Members

7. *Chemistry International* (*CI*). At present all Affiliates and contributors whose names are listed in the IUPAC Handbook receive *CI*, and it is assumed that this practice will be continued. It has been suggested that changes to *CI* are necessary to reflect, in part at least, what Affiliates would like to see and what is missing at present. Have you specific suggestions concerning the format, contents and frequency of publication of *CI*? For example, are there too many photographs of individuals or are such photographs relevant? Are the contents of wide interest? Are more news and views from Member Countries desirable? Would changing the quality of paper or quality of the cover be acceptable if such changes decreased production costs?

8. Other benefits for IUPAC Affiliates include reduced

prices for IUPAC publications, and reduced registration fees for IUPAC-sponsored conferences and symposia. (Reduced registration at one conference probably pays for the Affiliate Membership fee!). Can you suggest other benefits which might prove attractive to current and prospective Affiliate Members?

D. Other suggestions

9. Do you have any other suggestions for improvement of the Affiliate Membership Programme?

Please direct your replies to: Prof. J.W. Lorimer Department of Chemistry The University of Western Ontario London, Ontario N6A 5B7, Canada Fax: +1 (519) 661 3022; e-mail: lorimer@julian.uwo.ca

We should like to have your replies by *29 February 1996* as input to a full report which CAM hopes to complete for the meeting of the Executive Committee on 19–22 April 1996.

As Affiliates and participants in IUPAC programmes, your replies to the above questions on an important activity of IUPAC constitute advice which will be valued highly by CAM. Modification of the Affiliate Membership Programme forms part of the continuing efforts of the Bureau to make IUPAC more efficient and, at the same time, to increase the value of its contributions to the chemical community. We need your help in this task.

J.W.Lorimer
Dept. of Chemistry
The University of Western Ontario

Provisional Recommendations

IUPAC seeks your comments

In this section we publish synopses of IUPAC's latest provisional recommendations on nomenclature and symbols. All comments on these recommendations are welcome and will be taken into consideration. The final revised versions are published in *Pure and Applied Chemistry* and synopses of these are published in *Chemistry International* as recent reports.

If you would like to comment on the provisional recommendations please write to your nearest national/regional centre requesting a copy of the full report. Copies are not available from the IUPAC Secretariat. The most recent list of the national/regional centres appeared in *Chem. Intl.* 1995, **17**, 141.

Nomenclature for chiral chromatography

In recent years there has been considerable interest in the synthesis and separation of enantiomers of organic compounds because of their importance in the pharmaceutical industry. Frequently, the methods used for the separations or for monitoring the progress of a chiral reaction are chromatographic, with either liquids, gases, or supercritical fluids as the mobile phase. More recently, capillary electrophoresis has been added as an analytical chiral separation method.

These applications have lead to a number of terms and expressions in addition to those recently proposed for the chemistry and physical properties of chiral compounds. This present Nomenclature provides the description and definition for additional terms particularly related to analytical separation methods, the enantiomeric purity of the products and of their formation.

Comments on these recommendations are welcome and should be sent by 31 May 1996 to:

Prof. Roger M. Smith, Department of Chemistry. Loughborough University of Technology, Loughborough Leicestershire, LE11 3TU, UK.

Chemically modified electrodes: recommended terminology and definitions

Chemically modified electrodes (CME) comprise a relatively modern approach to electrode systems that find utility in: (i) a wide spectrum of basic electrochemical investigations, including the relationship of heterogeneous electron transfer and chemical reactivity to electrode surface chemistry, electrostatic phenomena at electrode surfaces, and electron and ionic transport phenomena in polymers, and (ii) the design of electrochemical devices and systems for applications in chemical sensing, energy conversion and storage, molecular electronics, electrochromic displays, corrosion protection and electro-organic synthesis.

Compared with other electrode concepts in electrochemistry, the distinguishing feature of a CME is that a generally thin film (from monomolecular to a few microns in thickness) of a selected chemical is bonded

or coated onto the electrode surface to endow the electrode with the chemical, electrochemical, optical, electrical, transport, and other desirable properties of the film in a rational, chemically designed manner.

In this report, we have attempted to identify and define the most widely used terminology in the growing field of CMEs and to recommend a particular term in cases where a multiplicity of terms has arisen over the past several years or where previously defined terms have taken on broadened meanings for the special cases of CMEs. It is expected that additional terms will be added to this lexicon in the future as new research directions evolve.

Comments on these recommendations are welcome and should be sent by 31 May 1996 to:

Prof. R.P. Buck Department of Chemistry, University of North Carolina at Chapel Hill, Venable Hall 045A, Chapel Hill, North Carolina 27599-3290, USA.

Classification and characterization of stationary phase for liquid chromatography—Part 1. Descriptive terminology

A wide range of stationary phases and column material have been developed over the years for liquid chromatography and it is important that these can be described accurately and unambiguously. The present paper, which is the first of a series planned for this area, proposes a number of terms to standardize the description of the stationary phase materials and their properties, and expands the list of terms given in General Nomenclature of Chromatography (*Pure Appl. Chem.* 1993, **65,** 819–872). It concentrates on the chemical properties and chromatographic role of the materials as many of the terms, used to describe their physical properties as particles, have been given in a recent paper on the characterization of porous solids (*Pure Appl. Chem.* 1994, **66,** 1739–1758).

Comments on these recommendations are welcome and should be sent by 31 May 1996 to:

Prof. Roger M. Smith Department of Chemistry Loughborough University of Technology Loughborough Leicestershire, LE11 3TU, UK.

Glossary of terms used in computational drug design

Computational drug design is a rapidly growing field which is now a very important component in the discipline of medicinal chemistry. At the same time, however, many medicinal chemists lack significant formal training in this field and may not have a clear understanding of some of the terminology used but need to grasp concepts, follow research results, define problems for, and utilize the findings of, computational drug design.

In this context, the IUPAC Medicinal Chemistry Section Committee felt that it would be useful to develop a glossary of terms used in computational drug design for easy reference purposes. Also there is the possibility that in different countries certain terms may not have the same meaning and in such a case there would be value in trying to establish an international definition standard.

Accordingly, a Working party of seven experts in this field was assembled and they have constructed a glossary of some 108 terms. Concise, but sufficient explanatory definitions have been formulated based on a variety of literature sources and some key references provided.

Comments on these recommendations are welcome and should be sent by 31 May 1996 to:

Dr. H. van de Waterbeemd, F. Hoffmann-La Roche Ltd, Dept. PRPC 65/314, CH-4002 Basle, Switzerland.

Nomenclature, symbols, units, and their usage in spectrochemical analysis—XVIII. Laser-based molecular spectroscopy for chemical analysis—raman scattering processes

This report is the 18th in a series on Spectrochemical Methods of Analysis issued by IUPAC Commission V.4 (Spectrochemical and other Optical Procedures for Analysis). This particular report is concerned with Raman scattering processes, usually induced by laser, covering the visible, UV and near infrared spectral regions. Raman scattering can be divided into linear and nonlinear processes. However, due to their importance for chemical analysis, mainly linear Raman effects are treated.

Comments on these recommendations are welcome and should be sent by 31 May 1996 to:

Dr. D.S. Moore, Chemical Science and Technology Division, Los Alamos National Laboratory, Los Alamos, NM 87544, USA.

Names and symbols of transfermium elements

Recommendations for the names and symbols of the transfermium elements (atomic number 101–109) are presented along with the reasons for proposing them.

Comments on these recommendations are welcome and should be sent by 31 May 1996 to:

Prof. A.M. Sargeson, Research School of Chemistry, Australian National University, Canberra, ACT 0200 Australia.

IUPAC recommendations on names and symbols of transfermium elements

Naming new elements has always been a delicate matter. For example, many elements are named differently in different countries. A typical example is the element denoted with the symbol N which is called Nitrogen in the UK and USA, Stickstoff in Germany, Azot in Russia, and Azote in France. Further examples are the elements with symbols Na, which is called either Natrium or Sodium, and K, which is called Kalium or Potassium. There is thus some longstanding disorder in naming elements amongst various countries. However, in the past the various chemical communities have always been able to mutually agree on the symbols which are used to denote newly discovered element. Therefore, the same symbols are used to denote the same chemical compound or the same chemical reaction all over the world.

Unfortunately, this situation has changed with the so called 'transfermium' elements—elements with atomic number greater than 103. Most of these elements where initially discovered by teams of researchers from three countries (USA, Russia and Sweden). Later, the team from Sweden withdrew from this line of research and a team from Germany took up the challenge of synthesysing new elements. Unfortunately, the discoverers of these new heavy elements could, in some cases, neither agree on which of them were actually the discoverers, nor on the names of these elements. Under these circumstances, within the last 30 years, IUPAC had made many attempts to assist in solving this problem.

The first discussion on how to acheive consensus in the nomenclature of these elements took place in 1971 at the General Assembly in Washington, DC, USA. At that time, the Inorganic Chemistry Division came up with the proposal to name new transfermium elements in a systematic way based on their numbers in the periodic table rendered in Latin. However, the Council did not vote for this proposal. Later at Davos (1979), the Council did vote for such a system of naming new elements. However, it left the possibility for renaming the elements after the controversies concerning their discovery were eliminated.

Time pased, yet the teams that synthesize new transfermium elements still could not come to an agreement. Therefore in 1986, the IUPAC Bureau accepted an invitation from the International Union of Pure and Applied Physics (IUPAP) to participate in a joint working group, Transfermium Working Group (TWG), created with the aim of solving the matter of priorities in the discoveries of transfermium elements. TWG worked hard, they visited all three laboratories, Darmstadt in Germany, Dubna in Russia, and Berkeley in the USA, where the work on the synthesis of transfermium elements continues. After extensive discussions, at the initial stage with the participation of the laboratories involved, and at the final stage without their participation, the TWG prepared three documents: Part I—*Criteria that must be satisfied for the discovery of a new chemical element to be recognized*, Part II—*Introduction to discovery profiles*, and Part III—*Discovery profiles of the transfermium elements*. In Part III, TWG has summarized its conclusions on which team, or teams, should be considered as the discoverers of each transfermium element.

Part I of the TWG report has been published in *Pure and Applied Chemistry* 1991, **63**(6), 879–886. Parts II and III have been published in *Pure and Applied Chemistry* (*PAC*) 1993, **65**(8), 1757–1814, together with the responses from the three laboratories concerned (the report was sent to them before publication and their comments were requested by IUPAC) and final response of TWG to criticism expressed in the above mentioned responses. In this report, TWG stated that these responses have not changed their conclusions. After that, the IUPAC Executive Committee endorsed the report of TWG. IUPAP has already done the same.

Based on the conclusions of TWG, the President of IUPAC contacted the Chairman of the Commission on Nomenclature of Inorganic Chemistry (CNIC), asking him to discuss the matter of naming transfermium elements taking into consideration the conclusions of TWG.

The recommendations of the CNIC were endorsed by the Inorganic Chemistry Division Committee and Interdivisional Committee on Nomenclature and Symbols (IDCNS) and then endorsed unanimously by the IUPAC Bureau at its meeting in Antwerp. In view of such unanimity, at this meeting, the Bureau decided to publish the recommendations in *PAC* as definitive. However, it was decided to indicate in this publication in *PAC* that the recommendations are still subject to approval by the IUPAC Council. After the recommendations, and their endorsement by the IUPAC Bureau, had became widely known, certain criticism concerning the recommendations and the procedure used to handle them by the Bureau, was expressed by a number of chemists.

It is the policy of IUPAC, before making decisions on the nomenclature issues, always to get as much agreement on them between the communities of chemists from various countries, as possible. Therefore, at its meeting on 11 August 1995, during the IUPAC General Assembly at Guildford, the Bureau decided to consider the recommendations published in *PAC* as provisional and to postpone the final decision of the IUPAC on the nomenclature of transfermium elements for two years until the General Assembly at Geneva in 1997.

K. I. Zamaraev
(President, IUPAC)

2nd International Symposium Molecular Order and Mobility in Polymer Systems, St. Petersburg, Russia, 21–24 May 1996

IUPAC SPONSORED

The Institute of Macromolecular Compounds of the Russian Academy of Sciences is continuing the series of St. Petersburg meetings on macromolecules. The Second International Symposium entitles, Molecular Order and Mobility in Polymer Systems, will be held in St. Petersburg next May.

The aim of the Symposium is to discuss the modern problems of thermodynamics, structure and properties of partly ordered polymer systems. Attention will be paid to the equilibrium properties of polymer systems. However, problems of dynamics will not be excluded. The topics of the Symposium will cover behaviour of polymer chains in different polymer systems, including:

- Macromolecules in solutions, melts and networks oriented and stretched in strong external fields;
- Liquid crystalline polymers;
- Block-copolymers;
- Polymer layers and micelles.

Both experimental data and the results of theoretical simulations will be presented. The Symposium programme will include 20 invited lectures of about 25 min, there will also be poster sessions.

A view on the Neva and Peter-and Paul's Fortress from the windows of the House of Scientists.

English will be the working language of the Symposium, there will be no simultaneous translation facility.

The registration fee is USD300 for regular participants who register before 1 March 1996, USD330 after this date, and USD100 for students who register before 1 March 1996, USD110 after this date. The registration fee for accompanying persons is USD50. As recommended by IUPAC, to facilitate the participation of scientists from Eastern European countries at IUPAC-Sponsored conferences, the registration fee for these scientists will be reduced to that of the students.

Address for correspondence: Prof. T.M. Birshtein, Institute of Macromolecular Compounds, Bolshoy pr. 31, St. Petersburg 199004 Russia. Tel.: (812) 213 1070 and 218 8744; Fax: (812) 218 6869; E-mail: birshtei@macro.lgu.spb.su

How to apply for IUPAC sponsorship

To apply for IUPAC sponsorship, conference organizers should write to the IUPAC Secretariat (see inside back cover for address) requesting an Advanced Information Questionnaire (AIQ). Completed AIQs should be returned to the Secretariat preferably 2 YEARS and at least 12 months before the conference. Late applications will not be considered. Further information on granting of IUPAC sponsorship was published in *Chem. Intl.* **14**, 203 (1992).

IUPAC International Symposium on Macromolecular Condensed State (ISMCS'96), Beijing, China, 20–25 August, 1996

IUPAC SPONSORED

Polymer chemistry and physics has now developed to a mature science. However, there remain many problems of a basic or fundamental nature which remain to be understood—this is particularly so at the molecular level. The inter-chain and inter-segmental interactions play an important role in the macromolecular condensed state. The purpose of this Symposium is to exchange and discuss ideas and new results on some basic issues in the molecular understanding of the macromolecular condensed state. It is hoped that the Symposium will give a new impetus to investigations of this important state of matter.

Main topics for discussion at the Symposium:

- The process of molecular chain condensation—solid or film formation from dilute polymer solutions;
- Polymeric liquid crystalline state;
- Chain entanglement in the amorphous state;
- The nature of glass transition and sub T_g annealing;
- Orientation, relaxation and crystallization from the amorphous state;
- Single chain particle-glasses and single crystals;
- Compatability and phase separation of polymer blends;
- Crystallization of polymer blends.

English will be the working language of the Symposium, there will be no simultaneous translation facility.

The registration fee is USD300 for regular participants and USD180 for graduate students. The registration fee for accompanying persons is USD100.

Address for correspondence: Prof. Xigao Jin, Institute of Chemistry, Chinese Academy of Sciences, PO Box 2709, Beijing 100080 China. Tel.: +8610 256 4829; Fax: +8610 256 9564; E-mail: huangsl@rose.cnc.ac.cn

10th International Cereal and Bread Congress, Porto Carras (Chalkidiki), Greece, 9–12 June, 1996

The Tenth International Cereal and bread Congress, *Cereals '96 The Source and the Future of Civilization*, is under the aegis of the International Association of Cereal Science and Technology (ICC), the Greek Minister of Agriculture and the Greek Ministry of Culture.

Address for correspondence: Secretariat, 10th International Cereal and Bread Congress, Ministry of Agriculture, Att: Dr. G. Bakayiannis, 5, Acharnon Street, GR 10176 Athens, Greece. Tel.: +30 1 524 4851; Fax: +30 1 524 8584.

15th International CODATA Conference (CODATA '96) 'Scientific Data in the Age of Networking', Tsukuba, Japan, 29 September–3 October, 1996

CODATA, the Committee on Data for Science and Technology, is an interdisciplinary scientific committee of the International Council of Scientific Unions, established in 1966 it seeks to improve the quality, reliability, management and accessibility of data of importance to all fields of science and technology.

The 15th CODATA Conference will be held at the Auditorium of the Agency of industrial Science and Technology, Tsukuba, Japan. The sessions will be organized around:

- Advanced theory and technology of computer science;
- Data handling on the information highway and data dissemination by multimedia;
- Advanced application for value creation;
- Intellectual property and copyright; publicity and security of data;
- Education and training;
- Other topics on data for environmental, geoscience, and materials science, molecular and medical biology, systematics, physics and chemistry.

Obtaining information via Internet

Information about the conference including exhibition news and a directory of Institutes located in Tsukuba are available on the Internet WWW pages located at:
http://www.race.u-tokyo.ac.jp/codata96
http://www.cisti.nrc.ca/codata/codata96

Information about CODATA may be obtained from the CODATA Secretariat: Mme P. Glaeser, Executive Director, 51 Blvd de Montmorency, 75016 Paris, France. codata@paris7.jussieu.fr

8th International Conference on Phenothiazines and Structurally Related Psychotropic Compounds, Jaipur, India, 26–29 February, 1996

IUPAC SPONSORED

The 8th International Conference on Phenothiazines and structurally related psychotropic compounds has been organized in the Chemistry Department of Rajasthan University in Jaipur, India. Jaipur, known as the Pink City, is the capital of Rajasthan State and is located about 300 km from Dehli.

The conference will consist of plenary and invited lectures, together with oral and poster presentations. The official language of the conference will be English. This scientific scope of the conference will cover the following topics:

1 Physical and chemical aspects
2 Analytical aspects and advances in assay methodology
3 Advances in drug metabolism
4 Toxicological aspects
5 Progress on mode and site of action
6 Clinical pharmacology and structural activity relationships
7 Drug interactions with other drugs or macromolecules and the therapeutic complications
8 Present and future in microbiology and cancer.

Registration fees will be USD250 for participants and delegates, and USD100 for students and accompanying persons. All correspondence should be addressed to :

Dr. R.R. Gupta, 10A Vasundhara Colony, Tonk Road, Jaipur - 302018 India. Tel.: (141) 512694; Fax: (141) 515367.

10th International Biotechnology Symposium (IBS), Sydney, Australia, 25–30 August 1996

IUPAC SPONSORED

The 10th IBS will be held in the Sydney Convention

Center, Darling Harbour, Australia.

A number of symposia will be held:

1 Frontiers in polypeptide production
2 Frontiers in the production of metabolites
3 Biocatalysis and biotransformation
4 Integrated bioprocesses
5 Downstream processing
6 Bioinstrumentaion and bioinformatics
7 Policy issues in biotechnology
8 Environmental biotechnology
9 Agriculture and food biotechnology
10 Gene therapy and tissue engineering
11 Antibody engineering and applications
12 Genetically engineered vaccines

For further information, please contact: 10th IBS'96 Symposium Secretariat, PO Box 128, Sydney NSW 2001, Australia. Tel.: (61) 2 262 2277; Fax: (61) 2 262 2323; E-mail: veckels@tourhosts.com.au

International Conference on Environmental Biotechnology, Massey University, Palmerston North, New Zealand, 1–4 September, 1996

IUPAC
SPONSORED

The application of biotechnology in pollution abatement is extensive and the number of engineers, scientists and researchers with specific interests in biotechnology for pollution control continues to increase. The biological treatment of waste streams has been the major technology of waste treatment. The biological treatment of toxic and inhibitory pollutants in liquids and soil media is becoming increasingly considered as are the bioscrubbers for the treatment of gaseous emissions.

It is proposed that an international conference focusing on the biotechnological applications in pollution prevention, minimization and mitigation, and addressing topics ranging from molecular biotechnology to bioreactor analysis will provide an excellent platform to review the developments in this rapidly advancing field. This conference will follow the 10th International Biotechnology Symposium (IBS), Sydney, Australia, 25–30 August 1996.

The conference will comprise a plenary session and three technical sessions run in parallel, each day. The conference themes of advances in environmental biotechnology include:

1 Biotechnological approaches to waste minimization
2 Biodegradable materials and life cycle analysis
3 Biodegredation mechanisms
4 Molecular biotechnology
5 Anthropocentric pollutants in the environment and their impact
6 Ecology of biotreatment systems
7 Biological treatment of solid wastes
8 Biological treatment of toxic pollutants
9 Bioprocess development and characterization
10 Bioreactors: design and optimization
11 Modelling and control of biotreatment processes

The registration fee, if received before 31 July 1996, will be NZD560 and NZD600 if received after 31 July 1996. This registration fee includes attendance at technical sessions, a bound copy of the proceedings, cocktails, lunches and the conference dinner.

Please direct all correspondence to: Conference Secretary, Environmental Biotechnology Conference, Process & Environmental Technology Department, Massey University, Palmerston North, New Zealand. Tel.: (64) 6 350 5351; Fax: (64) 6 350 5654; E-mail: g.f.withers@massey.ac.nz

5th International Workshop on Positron and Positronium Chemistry (PPC5), Lillafüred, Hungary 9–14 June, 1996

IUPAC
SPONSORED

The scientific organizers of this meeting are the Eötvös University, Budapest and the KFKI Research Institute for Particle and Nuclear Physics of the Hungarian Academy of Sciences.

As in past meetings, the subject matter of the workshop will encompass a broad range of experimental and theoretical topics:

1 Positrons and positronium in liquids
2 Chemical reactions of positronium
3 Chemical applications of positron beams
4 Surface structure and adsorbates
5 Polymers
6 Biological and micellar systems
7 $2\gamma - 3\gamma$ annihilation
8 Material characterization
9 Data evaluation and standardization
10 Instrumentation, etc.

A series of 45 min invited plenary lectures will be coupled with contributed oral lectures of 20 min duration. Poster sessions will provide ample time for informal exchange of scientific views. Topics of special interest will serve themes

for round table discussions—suggestions are welcome.

Lillafüred is a small mountain resort about 180 km north-east of Budapest, the workshop will take place in the Hotel Palace. Budapest is easily reached by plane, train or car. Participants can proceed from Budapest to Miskolc (the second city of Hungary) by intercity trains. A bus service between Miskolc and Lillafüred (10 km) will be provided by the organizers at the beginning and end of the workshop.

The organizers will do their best to keep fees and prices competitive. The registration fee will be about DEM300. Accommodation and meals will be offered in Hotel Palace, Lillafüred. Full board from 9–14 June will be about DEM480–530.

For scientific correspondence, please contact: Prof. Béla Lévay, Institute of Chemistry, Eötvös University, H-1518 Budapest 112, P.O. Box 32, Hungary. Fax: (36-1) 209 0598; E-mail: ppc5@rmk530.rmki.kfki.hu and levaybela@ludens.elte.hu

Dr. Zsolt Kajcsos KFKI Research Institute, H-1525 Budapest 114, PO Box 49, Hungary. Fax: (36-1) 169 6567; E-mail: ppc5@rmk530.rmki.kfki.hu and kajcsos@rmk530.rmki.kfki.hu

Conference Calendar

1996

Phenothiazines and related psychotropic compounds

26–29 February
8th International Conference on Phenothiazines and Structurally Related Psychotropic Compounds. Jaipur, India.
Dr. R. R. Gupta, 10A Vasundhara Colony, Tonk Road, Jaipur-30218, India. Tel.: +91 (141) 512694; Fax: +91 (141) 515367.

Chemical physics for the 21st century

16–19 April
International Conference on Chemical Physics on the Border of the 21st Century. Moscow, Russia.
Prof. V. I. Goldanskii, Semenov Institute of Chemical Physics, Russian Academy of Sciences, Kosygin Street 4, Moscow 117977, Russia.

Molecular order in polymers

21–24 May
2nd International Symposium on Molecular Order and Mobility in Polymer Systems. St. Petersburg, Russia.
Prof. T. M. Birshtein, Institute of Macromolecular Compounds, Russian Academy of Sciences, Bolshoy pr. 31, St. Petersburg, 199004 Russia.

Free-radical polymerization

26–31 May
2nd International Symposium on Free-Radical Polymerization: Kinetics and Mechanism. Santa Margherita Ligure, Genoa, Italy.
Prof. S. Russo, Department of Chemistry, University of Sassari, Via Vienna 2, I-07100 Sassari, Italy. Tel.: +39 (79) 229556; Fax: +39 (79) 229559.

Mycotoxins and phycotoxins

27–31 May
9th International Symposiums on Mycotoxins and Phycotoxins. Rome, Italy.
Dr. Marina Miraglia, Instituto Superiore Sanità, Food Department, Viale Regina Elena, 299, I-00161 Rome, Italy. Tel.: +39 (6) 4990, ext. 377; Fax: +39 (6) 4451767.

Protein folding

17–20 June
International Symposium on Theoretical and Experimental Aspects of Protein Folding. San Luis City, Argentina.
Dr. J. Vila, IMASL-Universidad Nacional de San Luis, Ejército de Los Andes 950, 5700 San Luis, Argentina.

Oxidation of polymers

24–28 June
11th Conference on Polymers Thermal and Photo-induced Oxidation of Polymers and its Inhibition in the upcoming 21st Century. High Tatras, Slovak Rrepublic.
Prof. L. Rychlá, Polymer Institute, Slovak Academy of Sciences, Dubravská cesta 9, 842 36 Bratislava, Slovak Republic.

Surface forces

25–29 June
11th International Conference on Surface Forces. Moscow, Russia.
Dr. L. B. Boinovich, Institute of Physical Chemistry, Leninsky Prospect 31, 117915, Moscow, Russia.

Organic synthesis

30 June–4 July.
11th International Conference on Organic Synthesis. Amsterdam, Netherlands.
Conference Secretariat ICOS - 11, PO Box 1558, 6501 BN Nijmegen, Netherlands. Tel.: +31 (80) 234471; Fax: +31 (80) 601159.

Catalysis

30 June–5 July.
11th International Congress on Catalysis. Baltimore, USA.
Prof. Gary L. Haller, Department of Chemical Engineering, Yale University, PO Box 208286, New Haven, CT 06520-8286, USA. Tel.: +1 (203) 432 4378; Fax: +1 (203) 432 4387.

Organometallic chemistry

7–12 July
17th International Conference on Organometallic Chemistry. Brisbane, Australia.
Prof. C. Raston, Department of Chemistry, Monash University, Clayton, VIC 3168, Australia.

Chemical education

14–19 July
14th International Conference on Chemical Education - Chemistry: Expanding The Boundaries. Brisbane, Australia.
Dr. W. Beasley, Graduate School of Education, The University of Queensland, Brisbane, Queensland 4072, Australia.

Sweeteners

14–20 July
International Symposium on Sweeteners. Jerusalem, Israel.
International Symposium on Sweeteners, PO Box 50006, Tel-Aviv 61500, Israel. Tel.: +972 (3) 5140014; Fax: +972 (3) 5175674 or 5140077; E-mail: 100274.2665@compuserve.com

(Bio)degradable polymers

15–18 July
37th Microsymposium on Macromolecules (Bio)degradable Polymers: Chemical, Biological and Environmental Aspects. Prague, Czech Republic.
Dr. B. Valter, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám 2, 162 06 Prague, c-Petriny, Czech Republic.

Photochemistry

21–26 July
16th Symposium on Photochemistry. Helsinki, Finland.
Prof. J. Wirz, Institut für Physikalische Chemie, Universität Basel, Klingelbergstr. 80, CH-4056 Basel, Switzerland.

Solubility phenomena

22–25 July
7th International Symposium on Solubility Phenomena. Leoben, Austria.
Dr E. Königsberger, Symposium Secretary, Abteilung für Physikalische Chemie, Montanuniversität Leoben, A-8700 Leoben, Austria. Fax: +43 (3842) 402308; E-mail: koenigsb@unileoben.ac.at

Macromolecules

4–9 August
36th International Symposium on Macromolecules. Seoul, Republic of Korea.
Dr. Kwang Ung Kim, Secretariat of IUPACMACRO SEOUL'96, Division of Polymers, Korea Institute of Science & Technology, PO Box 131 Cheongryang, Seoul 130-650, Korea. Tel.: +82 (2) 957 6104; Fax: +82 (2) 957 6105; E-mail: iupac@kistmail.kist.re.kr

Excitonic processes

14–17 August
2nd International Conference on Excitonic Processes in Condensed Matter (EXCON '96). Bad Schandau, Saxonia, Germany.
Prof. M. Schreiber, Faculty of Natural Sciences, Technische Universität Chemnitz-Zwickau, D-09107 Chemnitz, Germany.

Coordination chemistry

18–23 August
31st International Conference on Coordination Chemistry. Vancouver, Canada.
31st ICCC Secretariat, UBC Conference Centre, 5961 Student Union Boulevard, Vancouver, BC, Canada V6T 2C9. Tel.: +1 (604) 822 1050; Fax: +1 (604) 822 1069.

Macromolecular condensed state

20–25 August
International Symposium on Macromolecular Condensed State. Beijing, China.
Prof. X. Jin, Institute of Chemistry, Chinese Academy of Sciences, PO Box 2709, Beijing 100080, China. Tel.: +86 (1) 02564829; Fax: +86 (1) 02569564; E-mail: huangsl@rose.cnc.ac.cn

Physical organic chemistry

25–29 August
13th International Conference on Physical Organic Chemistry. Seoul, Republic of Korea.
Prof. J. Suh, Department of Chemistry, Seoul National University, Seoul 151-742, Republic of Korea. Tel.: +82 (2) 8862184; Fax: +82 (2) 8743704; E-mail: jhsuh@cd4680.snu.ac.kr

Biotechnology

25–30 August
10th International Biotechnology Symposium. Sydney, Australia.
10th IBS '96 Symposium Secretariat, PO Box 128, Sydney, NSW 2001, Australia. Tel.: +61 (2) 2622277; Fax: +61 (2) 2622323; E-mail: veckels@tourhosts.com.au

Chemical thermodynamics

25–30 August
14th IUPAC Conference on Chemical Thermodynamics. Osaka, Japan.
Prof. M. Sorai, Executive Secretary of ICCT-96, Microcalorimetry Research Center, Faculty of Science, Osaka University, Toyonaka, Osaka 560, Japan. Tel.: +81 (6) 8505523; Fax: +81 (6) 8505526 (or 5288). E-mail: icct96@chem.sci.osaka-u.ac.jp

Environmental biotechnology

1–4 September
International Conference on Environmental Biotechnology. Palmerston North, New Zealand.
Conference Secretary, Environmental Biotechnology Conference, Process & Environmental Technology Department, Massey University, Palmerston North, New Zealand. Tel.: +64 (6) 3505351; Fax: +64 (6) 3505654. E-mail: g.f.withers@massey.ac.nz

CHEMRAWN IX

1–6 September
Sustainable Production, Use, Disposal and Recycling of Materials. Seoul, Korea.
Organizing Committee & Secretariat, IUPAC CHEMRAWN IX, Tongwon B/D 6th Floor, 128-27 Tangju-dong, Chongno-ku, Seoul 110-071, Korea.

Euroanalysis IX

1–7 September
Euroanaysis IX. Bologna, Italy.
Prof. L. Sabbatini, Dipartimento di Chimica, Università di Bari, Via Orabona 4, 70126 Bari, Italy. Tel.: +39 (80) 5442020/16/14; Fax: +39 (80) 5442026.

Characterization of porous solids

15–18 September
4th International Symposium on Characterization of Porous Solids (COPS-IV). Bath, UK
Elaine Wellingham, Conference Secretariat, Field End House, Bude Close, Nailsea, Bristol, BS19 2FQ, UK. Tel. and Fax: +44 (1275) 853311.

Chemistry of natural products

15–20 September
20th IUPAC Symposium on the Chemistry of Natural Products. Chicago, USA.
IUPAC Symposium Headquarters, 5999 Butterfield Road, Hillside, Chicago, IL 60161, USA.

Multiphoton processes

30 September–4 October
7th International Conference on Multiphoton Processes. Garmisch Partenkirchen, Germany.
Prof. P. Lambropoulos, Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, D-85748 Garching, Germany.

Step growth polymerization

End-September
International Symposium on Step Growth Polymerization, Related Processes and Materials. Paris, France.
Dr. B. Sillion, Laboratoire de Chimie Macromoléculaire, Université Pierre et Marie Curie, 4 place Jussieu, 75252 Paris Cédex 05, France. Tel.: +33 (1) 78022078; Fax: +33 (1) 78022010.

1997

Thermodynamics

5–8 January
International Symposium on Chemical and Biological Thermodynamics. Amritsar, India.
Prof. D. V. S. Jain, Department of Chemistry, Panjab University, Chandigarh 160014, India. Tel.: +91 (172) 541435; Fax: +91 (172) 541409; E-mail: dvs-jain@imtech ernet.in

Bioorganic chemistry

1–6 June
4th International Symposium on Bioorganic Chemistry. Biarritz, France.
Prof. A. Marquet, Université Paris URA CNRS 493, Laboratoire de Chimie Organique Biologique, Tour 44/45 - 4 Pl. Jussieu, 75252 Paris Cedex 05, France.

Recycling of polymers

14–17 July
38th Microsymposium on Macromolecules, Recycling of Polymers. Prague, Czech Republic.
Dr. B. Valter, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám. 2, 162 06 Prague, 6–Petriny, Czech Republic.

International Union of Pure and Applied Chemistry (IUPAC)

IUPAC

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The International Union of Pure and Applied Chemistry (IUPAC), formed in 1919, is a voluntary non-governmental, non-profit association of organizations, each of which represents the chemists of a member country.

Its objectives are:

- to promote continuing co-operation among the chemists of the member countries;
- to study topics of international importance to pure and applied chemistry which need regulation, standardization, or codification;
- to co-operate with other international organizations which deal with topics of a chemical nature;
- to contribute to the advancement of pure and applied chemistry in all its aspects.

The membership of IUPAC presently comprises 40 countries, each represented by a national organization, such as an academy of science or research council.

National Adhering Organizations

Academy of Scientific Research and Technology **(Arab Republic of Egypt)**
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Australian Academy of Science **(Australia)**
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Chemistry International

IUPAC

1996, Vol. 18, No. 1 (January)

1 Istanbul 1995

8 Thirteen million—and still growing

10 The consequnces of poor mixing

13 The Committee on Teaching of Chemistry (CTC): an appraisal
Krishna V. Sané

21 PAC Review

25 Recent Reports

30 Affiliate Affairs

31 The Affiliate Membership Programme: Input from readers of *Chemistry International*

32 Provisional Recommendations

35 Conferences

38 Conference Calendar

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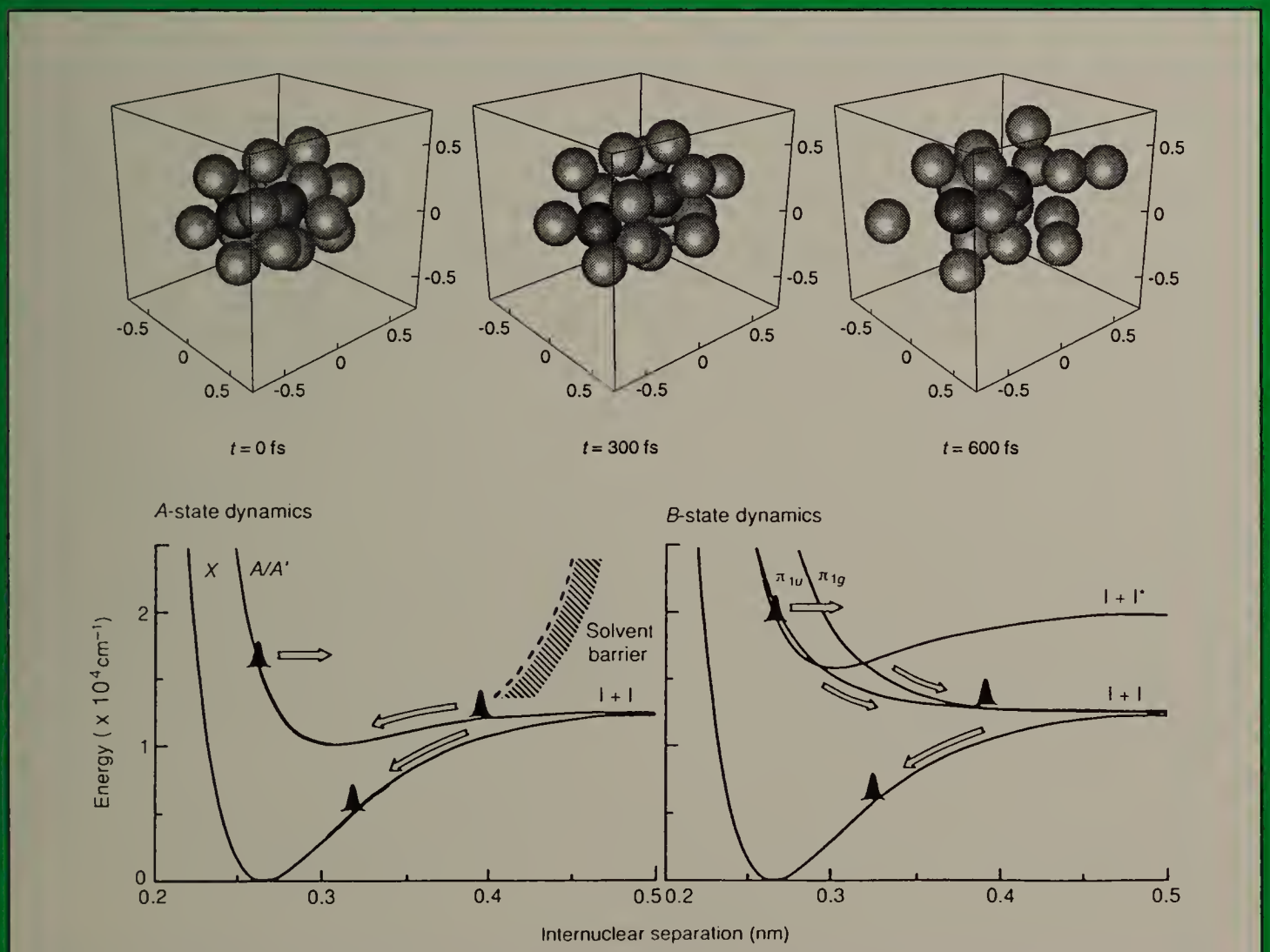

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The news magazine of the International Union of Pure and Applied Chemistry (IUPAC)

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Front cover: Femtosecond dynamics of an elementary reaction ($I_2 \rightarrow 2I$) in solvent (Ar) cages (see page 61).

International Union of Pure and Applied Chemistry

International Organization for Chemical Sciences in Development (IOCD)

A group of eminent research chemists from 15 countries gathered at UNESCO, Paris, in the spring of 1981, determined to find a way to assist fellow chemists in developing countries to overcome the barriers that hinder them from undertaking research on topics that would contribute to the development of their countries. The group decided to form a new nongovernmental international agency, **International Organization for Chemical Sciences in Development** (IOCD), registered in Belgium as a nonprofit organization.

Their plans called for this new agency to work along two principal lines in helping to overcome the barriers to research in developing countries. First, it would draw chemists in developing countries into collaboration in research with internationally recognised investigators from industrialised countries on development-related topics. Secondly, it would provide chemists from developing countries with the opportunity to receive hands-on instruction in research techniques through participation in laboratory workshops organized in developing countries.

These objectives would be pursued through Working Groups—an arrangement for linking chemists in Europe and North America with their colleagues in developing countries. At present, there are four active working groups in IOCD:

(1) IOCD Working Group on Fertility Regulation

Chairman: Dr Josef Fried,
Chemistry Department,
University of Chicago,
Chicago, Illinois, USA

Vice Chairman: Dr Stephen Matlin,
Commonwealth Secretariat,
London, UK

This working group is carrying out research on the chemistry and mechanism of action of new antifertility agents in the male. These agents are synthesised by chemists in developing countries who are members of the working group and then tested in a biological laboratory in the United States under the supervision of Prof. M. James Cosentino (Professor of Biology at Millersville University, Millersville, Pennsylvania, USA).

(2) IOCD Working Group on Tropical Diseases

Chairman: Dr Fred Opperdoes,
Research Unit for Tropical Diseases,
International Institute of Cellular & Molecular Pathology,
Brussels, Belgium

Vice Chairman: Dr Thomas Goodwin,
Chemistry Department,
Hendrix College,
Conway, Arkansas, USA

Here, chemists in developing countries synthesize compounds that are then tested as possible new chemotherapeutic agents in the treatment of tropical diseases such as malaria, filariasis, etc.

(3) Working Group on Plant Chemistry

Chairman: Dr Kurt Hostettmann,
Institut de Pharmacognosie et Phytochimie,
Universite de Lausanne,
Lausanne, Switzerland

Vice Chairmen: Dr Ermias Dagne,
Chemistry Department,
Addis Ababa University,
Addis Ababa, Ethiopia
Dr Patrick Moyna,
Facultad de Ciencias,
Montevideo, Uruguay

The Working Group on Plant Chemistry organizes laboratory workshops on simple bioassay techniques for natural products chemists (1990, Nairobi, Kenya; 1992, Accra, Ghana; 1994, Uruguay; (planned for 1996) Harare, Zimbabwe).

(4) Joint IUPAC/IOCD Working Group on Environmental Analytical Chemistry

IOCD and the International Union of Pure and Applied Chemistry (IUPAC) agreed in 1993 to form a joint working group on environmental analytical chemistry with emphasis on developing countries. The group is currently planning to organize workshops for analytical chemists in developing countries to assist them to take part in environmental monitoring. The Chairman of the joint working group is Dr Walter R. Benson, Bethesda, Maryland, USA.

Through being responsive to the opinions of the chemists in developing countries, IOCD has found additional ways of working with them in overcoming some

of the barriers to research. Thus, in 1992, IOCD invited directors of laboratories in Ethiopia, Kenya and Zimbabwe to consider the benefits of cooperating among themselves in providing research services to chemists in Africa. Accepting this challenge, the directors formed a network of cooperating laboratories and gave it the name **Network for Analytical and Biological Services in Africa** (**NABSA**). They designated Dr Berhanu Abegas, Chemistry Department, Addis Ababa University, Ethiopia (now at the Chemistry Department, University of Botswana, Gaborone, Botswana), to be network coordinator. From a UNESCO grant, IOCD contributed funds to NABSA to help meet the costs incurred by the participating laboratories in responding to the requests from African chemists. NABSA is currently seeking funds from other donors to help meet these operational costs.

Major innovations in IOCD's programme of activities

As the first of these major innovations, the IOCD Working Group on Plant Chemistry is organizing an International Symposium on Chemistry, Biological and Pharmacological Properties of African Medicinal Plants, Victoria Falls, Zimbabwe, 25–28 February 1996. The symposium will bring together scientists from African and other countries who are involved in the phytochemical investigation of African medicinal plants. Participants from both academia and industry will attend the symposium, which will feature 12 plenary lectures; 6 lectures from African speakers and 6 from nonAfrican speakers. In addition, there will be contributions in the form of oral presentations and poster sessions. Prior to the symposium, from 22 to 24 February 1996, IOCD is organizing a laboratory workshop in Harare, Zimbabwe, for natural products chemists in Africa, providing them with the opportunity to learn techniques for bioactivity-guided fractionation. Registration for the symposium is open to all chemists throughout the world, who will be charged a registration fee of USD400. The workshop is open only to African chemists, who are invited to apply to IOCD for a limited number of travel scholarships. Registration requests and applications for the travel scholarships should both be sent to Dr Hostettmann in Lausanne.

The second major innovation in IOCD's activities is the effort to create a new world-level agency, called the **Biotic Exploration Fund**, which will catalyze a major increase in bioprospecting in developing countries. It is IOCD's conviction that this large increase in bioprospecting, when coupled with effective conservation measures, can help these countries put a stop to the destruction of their biodiversity resources, with loss to all mankind of many potential new drugs and agro-products.

The Biotic Exploration Fund, the proposal of Professor Thomas Eisner—a chemical ecologist of Cornell University, will provide financial and technical assistance to developing countries to help them build the scientific and entrepreneurial capacity required for bioprospecting. Bioprospecting is an integrated action that includes: constructing an inventory of local plant and animal species; studying these species in relation to local tradi-

Members of the IOCD Working Group on Plant Chemistry plan future workshops in Africa and Latin America.

Meeting in the Priestly Room of the Chemists Club, New York City, on 19 May 1995, Memebers of the IOCD Working Group on Plant Chemistry reviewed outcomes of its previous workshops on simple bioassay techniquesa in Nairobi, Kenya (1990), Accra, Ghana (1992) and Montevideo, Uruguay (1994) and made plans for the next workshop in Harare, Zimbabwe, in February 1996.

Pictured left to right: Dr Berhanu Abegaz (Gaborone, Botsawa), Dr Patrick Moyna (montevideo, Uruguay) Vice Chairman, Dr Micheal Tempesta (Moss Beach, CA), Dr J.R. Plimmer (Columbia, MO), Dr Charles Weiss, Jr (Bethesda, MD), Dr Kurt Hostettmann (Lausanne, Switzerland) Chairman, Dr Walter R. Benson (Bethesda, MD) and Dr Maurice Iwu (Owerri, Nigeria).

tions and their possible use in curing local diseases or other potential us providing a reliable supply of extracts and chemicals for screening by appropriate commercial clients for worldwide pharmaceutical or chemical application; mobilizing national and international capital; negotiating with the world pharmaceutical and chemical industry; and dealing equitably with indigenous peoples.

IOCD initiated the work of establishing this Fund in July 1994 under a grant of USD10 000 from the US National Academy of Sciences. This enabled IOCD to convene the Strategy Meeting for a Bioprospecting Initiative, bringing 20 specialists in fields related to bioprospecting (ethnobotany, conservation, natural products chemistry, indigenous rights, etc.) together with Prof. Eisner to discuss his concept of the Biotic Exploration Fund. A key participant in the meeting was Dr Rodrigo Gamez, Director, National Institute for Biodiversity (INBio), Costa Rica, a laboratory that is demonstrating the coordinated scientific effort that Prof. Eisner considers essential to bioprospecting. The Biotic Exploration Fund will seek to establish laboratories similar in purpose to INBio in many developing countries. At the conclusion of the Strategy Meeting, the experts unanimously recommended establishment of the Biotic Exploration Fund as follows:

We support the establishment of a Biotic Exploration Fund to attract sustained additional resources to finance increased local scientific and technological capacity for bioprospecting in developing countries and to add to human knowledge regarding the usefulness of natural products in such a way as to:

(1) increase local research and value added as the basis for a local biotechnology industry;

(2) create incentives for the conservation of biodiversity resources;

(3) contribute to upholding the rights of indigenous peoples and to the equitable sharing of the benefits derived from the bioprospecting effort.

We further recommend that the effort begin with a set of prudently managed and carefully focused undertakings in different parts of the world and expand as its success warrants. It should include a substantial element of technical assistance in project development and in the skills needed to collaborate with the private commercial sector.

The John D. and Catherine T. MacArthur Foundation has just awarded IOCD a grant of USD25 000 for the extensive work of drawing up the structure and functions of the Biotic Exploration Fund. To help it undertake a task of this magnitude, IOCD has retained the services of a consultant, Dr Charles Weiss, former Science and Technology Adviser of the World Bank, and is also setting up an Advisory Committee of individuals with specialization in biodiversity and bioprospecting and representing the points of view of the many constituencies that are involved in both developed and developing countries: governments, scientists, universities, environmental organizations, indigenous peoples, modern and traditional biotechnology industry, foundations, aid agencies, conservation organizations, chemical and pharmaceutical companies, and venture capital companies. The initial meeting of the Advisory Committee will convene in September 1995 as an e-mail teleconference.

In order to take an experimental approach to selecting the structure and functions that are most suitable for the Fund, IOCD is organizing pilot projects in several African countries. IOCD has already identified candidates for these pilot projects and plans to carry out initial missions in the countries of the projects to assist local scientists and entrepreneurs to formulate proposals for bioprospecting projects that can be submitted to funding sources. IOCD hopes to attract sufficient funds (perhaps USD2–3m) to operate two or three pilot bioprospecting projects by 1997–1998.

Dr Lydia Rodriguez-Hahn, National Autonomous University of Mexica (UNAM) receives Syntex/IOCD Award for Chemical Excellence from IOCD President Emeritus Dr Glenn T. Seaborg at the 1991 National Meeting of the American Chemical Society in New York (pictured from left to right: Dr Robert Maybury, Executive Director, IOCD; Dr Lydia Rodriguez-Hahn and Dr Glenn T. Seaborg).

IOCD governance

IOCD is governed by an Executive Committee, comprising its President, Vice-President/Treasurer, and Executive Director. This committee can turn to a Senior Advisory Council comprising distinguished scientists, three of whom are Nobel Laureates.

The officers of IOCD are as follows:

President: Dr Jean-Marie Lehn,
Laboratoire de Chimie
Supramoleculaire,
Universite Louis Pasteur,
Strasbourg, France

Vice President & Treasurer:
Dr Elkan R. Blout,
Harvard School of Public Health,
Boston, Massachusetts, USA

Funding of IOCD's activities is through grants from individual donors and agencies such as foundations, government organizations and United Nations agencies (UNESCO, WHO, etc.). The IOCD affiliate, Organization for Chemical Sciences in Development, Inc. (OCDI), has 501 (c)(3) tax-exempt status with the US Internal Revenue Service.

Inquiries and requests for additional information about IOCD may be addressed to:

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Executive Director,
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Tel.: +1 703 845 9078; Fax: +1 703 845 9078,
E-mail: iocd@gwuvm.gwu.edu

Transport properties of R134a

Status of the round-robin on the transport properties of R134a (1,2,2,2-tetrafluoroethane)

Summary of an invited paper presented at the Twelfth Symposium on Thermophysical Properties, 19–24 June, 1994, Boulder, Colorado USA, and published, in full, as: M.J. Assael, Y. Nagasaka, C.A. Nieto de Castro, R.A. Perkins, K. Ström, E. Vogel, W.A. Wakeham; *International Journal of Thermodynamics* 1995, **16**(1), 63–78.

The paper contains a status report on an international project coordinated by the Subcommittee on Transport Properties of the Commission on Thermodynamics, of the Physical Chemistry Division, of IUPAC. The project has been conducted to investigate the large discrepancies between the results reported by various authors for the transport properties of R134a. The project has involved the remeasurement of the transport properties of a single sample of R134a in nine laboratories throughout the world in order to test the hypothesis that at least part of the discrepancy could be attributed to the purity of the sample. The full paper provides an intercomparison of the new experimental results obtained to date in this project for the viscosity and the thermal conductivity in both gaseous and liquid phases. The implications for future measurements of the transport properties of other refrigerants are significant.

Introduction

As is well known, the recognition that chlorine containing refrigerants have a detrimental effect upon the ozone layer has prompted a search for replacement materials that are less harmful to the atmosphere and resulted in consideration of the group of hydrofluorocarbons as suitable materials since they contained no chlorine. Among this group of compounds preliminary studies indicated that R134a (1,2,2,2-tetrafluoroethane) was a suitable substitute material for R12 which had been used traditionally in domestic refrigeration. This identification prompted a series of measurements in many laboratories throughout the world of the thermophysical properties of this material including equilibrium and transport properties. For the thermodynamic properties, the studies that ensued provided results that suffered from only mild inconsistencies which were resolved by a group working under the auspices of Annex 18 of the International Energy Agency. Their efforts have culminated in a definitive equation of state for R134a.[1] From the point of view of industrial design of refrigeration cycles, the thermodynamic properties of the refrigerant are more significant than the transport properties, so that work on the transport properties was initiated more slowly. In addition, it has transpired that the measurements suffered from far greater difficulties than had been expected.

At the Eleventh Symposium on Thermophysical Properties held in 1991, two independent reports of measurements of the viscosity of R134a were made and subsequently published by Diller *et al.*[2] and Fellows *et al.*[3] using different experimental techniques. The results of these two initial studies were very different; deviations of as much as 15% along the saturation line were apparent. This observation, combined with the increasing demand for viscosity and thermal con-

ductivity data, prompted new studies of this and several other potential replacement refrigerants including R32 and R125.

In November of 1992, a meeting of some of those interested in the thermophysical properties of refrigerants, in particular the transport properties, was held to review the situation with respect to new measurements. The conclusion of that meeting was that discrepancies remained that greatly exceeded the experimental uncertainties claimed by individual authors. It was therefore agreed to launch a project, which initially involved nine laboratories, to elucidate these problems. The present paper compares the results obtained on this round-robin sample among themselves and with results of earlier work.

Background

The saturated-liquid viscosity data[2–8] which were available for R134a in 1992 are shown in the deviation plot of Fig. 1. For comparison, the viscosity correlation of Krauss *et al.*[9] is used as the baseline in Fig. 1, even though it is not recommended for use below 290 K for viscosity (dashed baseline in figure). The uncertainty in the correlation[9] is estimated to be ± 5% as shown on the figure. The results included in the figure were obtained by a variety of techniques including capillary viscometers, vibrating-wire viscometers, and one oscillating quartz-crystal viscometer. The maximum deviation between the data sets[2–8] is 33% at 340 K and far exceeds the mutual uncertainty claimed by the authors, and the uncertainty of the baseline correlation. The results of Diller *et al.*[2] and Fellows *et al.*[3] appear to be systematically higher than the other results available in 1992. An examination[4] of the pressure dependence of the viscosity of R134a revealed a very much better agreement, although the absolute differences observed at saturation were maintained.

A review of the results for the dilute-gas-phase viscosity[10] showed deviations as much as 4% between the three data sets which were available at the time and obtained with two different types of viscometers. Again this deviation substantially exceeded the mutual uncertainty claimed by the authors.

The data sets for the viscosity of R32 and R125 were also examined[11] to determine whether this problem was specific to R134a. It was found that the discrepancies exceed 15%. The representation of the data of Oliveira & Wakeham[11] has been used as the baseline, and the figure includes the results of Ripple & Matar[5] with a capillary viscometer, Oliveira & Wakeham[11] with a vibrating-wire viscometer, and Diller & Peterson[12] with an oscillating quartz-crystal viscometer. It appears that the problem is a general one which is not limited to the case of R134a.

Viscosity discrepancies of this magnitude are at best embarrassing and at worst damaging to those interested in the viscosity of liquids. Possible explanations include improper working equations for one or more of the techniques, improper data analysis, carelessness on the part of the researchers, undetected equipment malfunctions, and differences in the chemical composition of the material studied.

For the thermal conductivity of R134a, the situation in 1992 was almost as serious in the liquid phase. Figure 2 contains a plot of the deviations of the thermal conductivity data[3,7,13–17] for liquid R134a along the saturation line from the correlation of Krauss *et al.*[9] which has been employed as the baseline. The uncertainty in the correlation[9] is estimated to be ± 5% for thermal conductivity as shown on the figure. Below 300 K the agreement between the data and the correlation is within ± 2.5%. This is interesting since the baseline correlation[9] is not considered valid below 240 K. The maximum deviations are about 20% in this case and occur near the critical temperature, but oddly this is the region where the correlation is considered valid. This value exceeds the mutual uncertainty claimed by the authors by almost an order of magnitude in some cases. In the vapour phase the few measurements available in 1992, mostly at low density, disagreed by as much as 15%.[9] Almost all of these data were obtained with the transient hot-wire method, although marginally different versions of the instrument were employed. These observations obviously threw doubt on the ability of some, if not all of the laboratories concerned, to make accurate thermal conductivity measurements, either because the experimental techniques were not understood, or because of inadequate sample purity or a combination of both.

Round-robin project

The issues raised in the study of R134a and other refrigerants such as R125 have potentially far wider consequences because it appeared that it was not possible to determine accurately even the viscosity of a liquid under ambient conditions (a task frequently assigned to undergraduate students). The threat to the credibility of future measurements of viscosity and thermal conductivity was significant. It is essential to identify the source or sources of the discrepancies between the results of various authors. As one part of this effort the problem of the purity of the samples must be addressed. Almost all experimenters had used samples supplied by different companies and the purity, as supplied, was not always specified. Furthermore, water was a potential impurity in samples of R134a, which even in trace amounts could have significant consequences for the viscosity of liquids and could also have a serious effect upon the electrical measurements associated with the transient hot-wire technique. The only manner in which sample

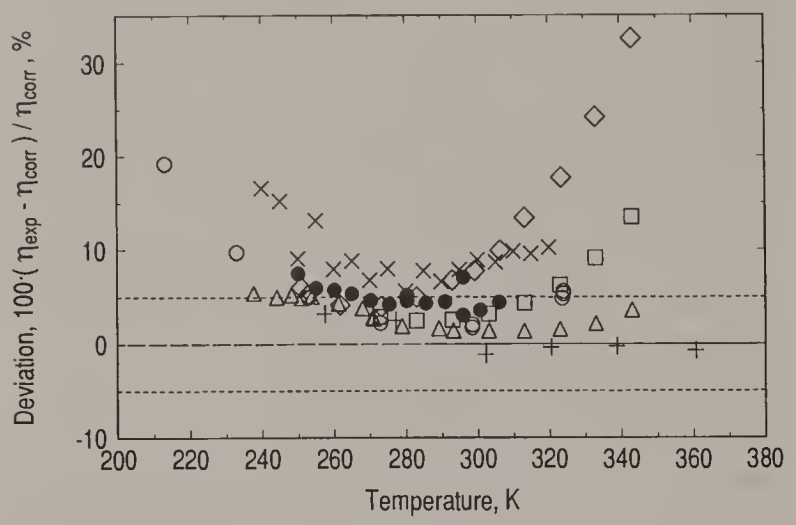

Fig. 1 Deviations of the viscosity of R134a in the liquid phase at saturation available in 1992 from the correlation of the results of Krauss *et al.*[9] (×) Diller *et al.*,[2] ( ) Fellows *et al.*,[3] ( ) Oliveira & Wakeham,[4] (●) Ripple & Matar,[5] (□) Kumagai & Takahashi,[6] (+) Ruvinski *et al.*,[7] (○) Okubo *et al.*[8]

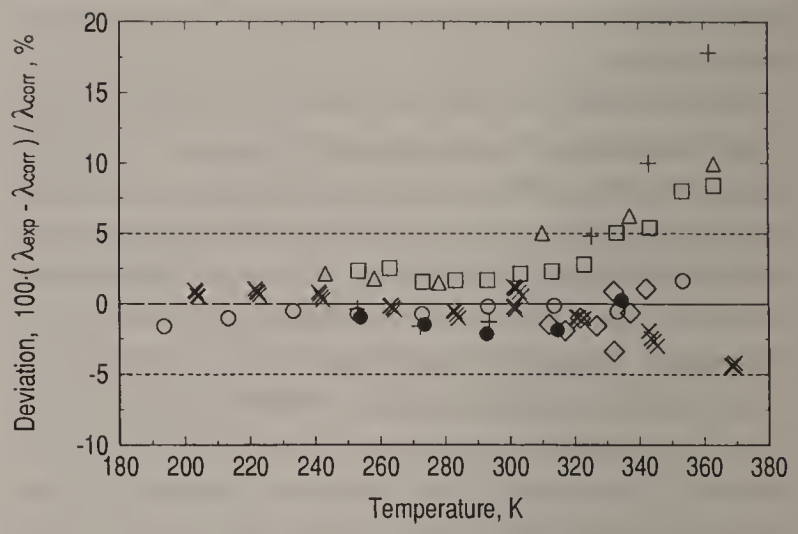

Fig. 2 Deviations of the thermal conductivity of liquid R134a along the saturation line available in 1992 from the correlation of Krauss *et al.*[9] (×)Laesecke *et al.*,[13] ( ) Ross *et al.*,[14] (□) Gross *et al.*,[15] (○) Ueno *et al.*,[16] ( ) Fellows *et al.*,[3] (+) Ruvinski *et al.*,[7] (●) Yata *et al.*[17]

purity could be investigated in a satisfactory manner was if various laboratories undertook measurements of the viscosity and/or thermal conductivity of R134a on the same sample with their own equipment. It was impractical to circulate the same sample amongst different laboratories since it is very time consuming and there is significant danger of loosing or contaminating the sample as it circulates. The present authors decided that a single source of supply of R134a should be selected and sufficient samples taken from that single source of supply to provide each laboratory with its own cylinder.

One company (ICI Chemicals and Polymers, UK) agreed to provide the single source of R134a and filled nine different cylinders from that same source, using procedures for pharmaceutical materials to ensure the cleanliness of the cylinders before use. The purity of the batch was confirmed by gas chromatography for organic impurities and the Karl–Fischer test for water. The purity of the batch was greater than 99.9%, and the principal impurity was R134 at a concentration of 850 ppm. Water was present at a concentration of 6 ppm. These nine cylinders of material were distributed in July 1993 to nine laboratories throughout the world who had volunteered to participate in the project in 1992. The laboratories were asked to conduct measurements of the transport properties using their preferred technique on the sample, taking care to maintain the purity of the sample and to recover the sample after use for subsequent analysis to ensure that the purity had not been degraded. All of the laboratories also agreed to use the equation of state for R134a reported by Tillner-Roth & Baehr.[1]

Summary

On the basis of this project, it is concluded that measurements made of the dilute gas viscosity by Wilhelm on the round-robin sample are consistent with the previous data of Dowdell & Matthews,[10] and Nabizadeh & Mayinger[18] who both used different samples of R134a. Purity was probably not a problem with these two viscosity data sets, and capillary measurements[10] agree with oscillating disk measurements (present work and Ref. 19) within the mutual uncertainty of the measurements. It would be desirable in the future to have other researchers measure the dilute-gas viscosity of the round-robin sample of R134a. No measurements of the dilute-gas thermal conductivity are available for comparison at this time.

The very large discrepancies that characterised early liquid phase viscosity results have not been repeated when an identical sample has been used. There is agreement within mutual uncertainty between liquid viscosity measurements made by means of the vibrating-wire technique and the falling-body technique using the round-robin sample. Additionally, the viscosity data on the round-robin sample and the previous data using the capillary technique[5–8] agree to within ± 3% at temperatures below 320 K. Also, the laboratories involved in the round-robin test of the viscosity have reproduced their earlier results within their estimated uncertainty. This would suggest that, while purity may have been, in part, responsible for the differences between the results observed earlier, there may be additional problems associated with the working equations or the operation of some of the instruments. Problems with measurement techniques will likely become more evi-

dent through examinations of results for several different fluids.

During the round-robin project, each researcher has taken extreme care during the measurements and the subsequent data analysis, using a carefully prepared sample of high purity. Despite these precautions, systematic (temperature dependent) deviations are observed with a magnitude of 5% in thermal conductivity measured by the transient hot-wire technique. Understanding of this discrepancy is crucial to the round-robin project and the credibility of the transient hot-wire technique. It is desirable to have researchers participate using a variety of experimental techniques including steady state technique and light scattering. Only three variants of the transient hot-wire technique are available at the time of this report. If the Yamada data set is excluded because of the electrical conduction problem reported in the Keio sample, the spread of values is generally about ± 1.5%, which is consistent with the claimed uncertainties of each of the researchers.

The round-robin project will continue for some time to allow other contributors to complete their measurements. This project will continue to examine problems in the measurement of the transport properties of refrigerants with future emphasis on the gas-phase thermal conductivity which has proved rather more difficult to measure than expected. The completion of this work should enhance the optimal application of new refrigerant materials, increase the understanding of the fluid state for a unique group of polar compounds, and establish the credibility and uncertainty of the techniques which are available to measure the transport properties of fluids.

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The IUPAC Solubility Data Project: Strategies and Coverage

J. W. Lorimer

IUPAC Commission V.8 (Solubility Data) adopted, at its formation in 1979, the goal of preparing compilations of all experimental determinations of solubility reported in the world's chemical literature and, where possible, evaluating these data critically. This enormous task is approached by considering systems of two or more well-defined components and producing printed volumes of compilations and critical evaluations of chemically related systems. The methodology used in compilations and critical evaluations has been described in *Chemistry International*,[1] in the *Series* itself (e.g. A.S. Kertes in the Foreword to Vol. 27/28) and recently in ref. (2). The results of these efforts are published as volumes in the IUPAC *Solubility Data Series*, and Volume 60 on 'Halogenated Methanes with Water' will have been published by late 1995. The Commission has received several requests to describe the strategy by which topics for volumes are chosen, with a view to complete coverage of the voluminous data which are to be found in the literature. This article describes the general principles underlying our strategy, and also is a report on the current status of the extent of coverage.

Prof. J. W. Lorimer

The Commission particularly encourages work on systems of widespread chemical interest and of practical concern to chemically related areas such as the environment, agriculture, human health and global climate change. However, in practice, the Commission must rely on the interests of those highly qualified contributors who wish to participate. In earlier years an extensive campaign was undertaken to recruit contributors, based on their expertise identified through their scientific publications. The task of compiling data proved to be much larger than expected initially. For example, in the important systems hydrogen in all solvents, sufficient material was found to produce a double volume 5/6. Since publication of that volume in 1981, sufficient newer references have appeared that a third updated volume could be produced. It has also proved difficult, especially in solid–liquid systems, to cover the area in a systematic way, again because of individual expertise and interests of contributors.

New contributors who have areas of special expertise, especially in the difficult area of complex salt systems, are always welcomed by the Commission. The list at the end of this contribution indicates that 48 scientists from a dozen countries have participated thus far in the *Solubility Data Series* as editors of and major contributors to volumes; at least an equal number have also contributed through various compilations and evaluations. Their names are to be found on the title pages of individual volumes.

Systems are classified in the first instance as belonging to one of three categories: gases in liquids, liquids in liquids, or solids in liquids. Within these categories, further classification is based on chemical similarities. Of the 60 volumes published or, in press at the time this note was prepared, 21 volumes (35%) contain data on gas–liquid solubilities, 8 volumes (13%) contain data on liquid–liquid solubilities, and 28 volumes (47%) contain data on solid–liquid solubilities. Three cumulative index volumes comprise the remaining 5%.

1. Gases in liquids

In this case, a strategy for covering the most important gases has been devised, and has been carried out systematically, for the most part. Simple monatomic and homonuclear diatomic gases in water and aqueous solutions are considered first, followed by heteronuclear diatomics and gases of increasingly complex molecular structure. With some classes, such as aliphatic amines, overlap with liquid–liquid systems occurs with propylamine and higher amines. The methods of reporting and evaluating data differ sufficiently for gases in liquids and for solids in liquids that division according to the most frequently encountered state of aggregation has been inevitable. The strategy is evident from the following list. Unless specified to the contrary (as in vols 21, 42, 45/46, 50), all volumes contain data on gases in all solvents which have been reported in the literature.

1.1 noble gases: vols 1, 2, 4
1.2 homonuclear diatomic and triatomic gases: vols 5/6, 7, 10, 12 (part)
1.3 hydrides (groups 13–15 of the periodic table, except carbon): Vol. 21
1.4 selected hydrocarbons: vols 9, 24, 27/28, 57
1.5 amines: Vol. 21 (part)
1.6 polyatomic gases containing oxygen: vols 8, 12 (part), 43, 50
1.7 sulfides, selenides: Vol. 32
1.8 halides: Vol. 42
1.9 gases in molten salts (special volume): Vol. 45/46

2. Liquids in liquids

Here, binary and multicomponent systems are considered in which the components are normally all liquids at room temperature and atmospheric pressure. However, because groups of chemically related systems are treated together, some systems containing gaseous or solid components are sometimes included as well. The first area of focus has been the solubility of organic liquids in water. Volumes have been organized for classes of organic compounds whose aqueous solubility is particularly relevant for scientific, industrial and environmental reasons, limited only by the areas of expertise of available contributors. While work is continuing on aqueous binary systems involving other classes of organic compounds, a start has been made on non-aqueous binary and ternary systems. For example, Vol. 56 concerns binary systems of alcohols with hydrocarbons, and a volume concerning alcohol–hydrocarbon–water systems is in preparation. The binary systems alcohol–water (Vol. 15) and alcohol–hydrocarbon provide systematic background material for evaluating the ternary systems. These systems were chosen mainly because of their importance in the manufacture of fuels. So far, eight volumes on liquids, or 13% of the total, have been published, as follows.

2.1 *binary systems containing water*

2.1.1 hydrocarbons in water: Vols 37, 38
2.1.2 alcohols in water: Vol. 15
2.1.3 esters in water: Vols 48, 49
2.1.4 halogenated aliphatics in water: Vol. 60
2.1.5 halogenated aromatics in water: Vol. 20

2.2 *binary non-aqueous systems*
2.2.1 alcohols with hydrocarbons: Vol. 56

3. Solids in liquids

Solids in liquids are divided into several groups: inorganic, organic and metal–organic salts, organic non-electrolytes. All salts (inorganic and organic) are classified according to the type of anion. Non-electrolyte organics are classified by structure. There are special volumes on pharmaceuticals, many of which are salts. Molten salts and alloys comprise a final group.

In a typical complex inorganic system, binary, ternary and higher systems may all be encountered. For binary systems, systematic methods of evaluation have been devised [2]. So far, evaluation of ternary systems has been relatively simple either because of the paucity of data or the occurrence of only one solid phase. Volumes in preparation will deal with more complex systems, such as systems containing common salts of the group 1 and 2 metals and ammonium.

3.1 *inorganic salts (for specific cations, see list of volumes)*
3.1.1 halides: vols 11, 22, 40 (part), 47
3.1.2 halates: vols 14, 30, 40, 44
3.1.3 oxyhalides: Vol. 40 (part)
3.1.4 perchlorates: Vol. 41
3.1.5 oxides, hydroxides: Vol. 23, 52
3.1.5 sulfites, selenites, tellurites: Vol. 26
3.1.6 nitrates: Vol. 13, 55
3.1.7 phosphates: Vol. 31
3.1.8 tetraphenylborates: Vol. 18
3.1.9 anions containing C, N and S: Vol. 3

3.2 antibiotics: Vols 16/17, 34, 35, 36
3.3 molten systems: Vols 25, 33, 51
3.4 organics: Vols 54, 58, 59
3.5 special systems (mercury): Vol. 29

In all three main categories, many projects are in progress, so that the above list will continue to grow in completeness and in coverage of important systems.

M. Salomon, Chairman of Commission V.8, Chairman-elect D. G. Shaw, and the Subcommittee Chairs, P. G. T. Fogg, F. W. Getzen and M.-T. Saugier-Cohen Adad, all provided helpful comments. Their contributions to this note and to the Solubility Data Project are acknowledged with thanks.

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Vol. 1. H. L. Clever, *Helium and Neon* (1979)
Vol. 2. H. L. Clever, *Krypton, Xenon and Radon* (1979)
Vol. 3. M. Salomon, *Silver Azide, Cyanide, Cyanamides, Cyanate, Selenocyanate and Thiocyanate* (1979)
Vol. 4. H. L. Clever, *Argon* (1980)
Vol. 5/6. C. L. Young, *Hydrogen and Deuterium* (1981)
Vol. 7. R. Battino, *Oxygen and Ozone* (1981)
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Vol. 15. A. F. M. Barton, ed., *Alcohols with Water* (1984)
Vol. 16/17. E. Tomlinson and A. Regosch, eds., *Antibiotics: 1,β-Lactam Antibiotics* (1985)
Vol. 18. O. Popovych, *Tetraphenylborates* (1981)
Vol. 19. C. L. Young, *Cumulative Index: Volumes 1–18* (1985)
Vol. 20. A. L. Horvath and F. W. Getzen, *Halogenated Benzenes, Toluenes and Phenols with Water* (1985)
Vol. 21. C. L. Young and P. G. T. Fogg, *Ammonia, Amines, Phosphine, Arsine, Stibine, Silane, Germane and Stannane in Organic Solvents* (1985)
Vol. 22. T. Mioduski and M. Salomon, *Scandium, Yttrium, Lanthanum and Lanthanide Halides in Non-aqueous Solvents* (1985)
Vol. 23. T. P. Dirkse, *Copper, Silver, Gold and Zinc, Cadmium, Mercury Oxides and Hydroxides* (1986)
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Vol. 39. C. L. Young, *Cumulative Index: Volumes 20–38* (1989)
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Vol. 60. A. L. Horváth and F. W. Getzen, *Halogenated Methanes with Water* (1995)

News

News Release from the Commission on Atomic Weights and Isotopic Abundances (II.1)

The Commission on Atomic Weights and Isotopic Abundances, at its meeting of the 38th IUPAC General Assembly in Guildford, UK, recommemded changes to the atomic weight values of five chemical elements based, in part, on the extensive evaluations of the natural isotopic variability of serveral elements.

Element	New atomic weight	Old atomic weight
B	10.811 ± 0.005	10.811 ± 0.007
C	12.011 ± 0.001	12.0107 ± 0.0008
Ce	140.115 ± 0.004	140.116 ± 0.001
Eu	151.965 ± 0.009	151.964 ± 0.001
Pt	195.08 ± 0.03	195.078 ± 0.002

The Commission also recommended small changes to the atomic weights of the following monoisotopic elements: Na, Al, P, Mn, Co, As, Cs, and Bi. The Commission recommended changes to the uncertainty values of the following monoisotopic elements: F, Sc, Rh, Pr, Tb, Ho, Tm, and Au.

STOP PRESS

IUPAC has just gone on-line on the Internet. Information about IUPAC and, eventually, news about IUPAC and its activities may be found on the world wide web at: http://chemistry.rsc.org/rsc/iupac.htm

To eliminate possible confusion in the reporting of isotopic abundance data on noncorresponding scales, the Commission recommends that:

1 $^{7}Li/^{6}Li$ ratios be expressed relative to L-SVEC lithium carbonate. Reporting of $^{6}Li/^{7}Li$ ratios be discontinued,

2 $^{37}Cl/^{35}Cl$ ratios be expressed relative to SRM 975 sodium chloride (Standard Reference Material from NIST). Reporting data relative to SMOC (Standard Mean Ocean Chloride) should be discontinued, and

3 $^{34}S/^{32}S$ ratios of all substances be expressed relative to VCDT (Vienna Canon Diablo Troilite) on a scale such that $^{34}S/^{32}S$ of IAEA-S-1 silver sulfide is 0.9997 times that of VCDT.

The Commission reaffirms its recommendation that: $^{18}O/^{16}O$ ratios of all substances be expressed relative to either VSMOW or VPDB on scales such that $^{18}O/^{16}O$ of SLAP is 0.9445 times that of VSMOW. In the absence of a direct calibration with the VSMOW-SLAP scale by analysis of reference water samples, analysts should indicate values of all isotopic fractionation factors used to determine the isotopic composition of a mineral or compound and should indicate the isotopic composition obtained for a reference material of the same mineral or compound.

Names and addresses

Full details (names, addresses, telephone/telex/Fax numbers and E-mail) of the officers of IUPAC bodies were published in *Chemistry International* 1995, **17**(6), 215–226. The IUPAC Secretariat have been notified of the following changes:

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Prof. Irina P. Beletskaya (Department of Chemistry, Moscow State University, Leninskie Gory, RU-119899 Moscow, Russia. Tel.: +7 095 939 3618; Fax: +7 095 939 1854) has been appointed Chairman of the Editorial Advisory Board of the Monographs on Chemistry for the 21st Century.

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Prof. Alan Sargeson (II.2), Department of Chemistry, Faculty of Science, Australian National University, Canberra, ACT 0200, Australia. Tel.: +61 6 249 2019/ 281 4704; Fax: +61 6 249 0760; E-mail: sargeson@rsc.anu.edu.au

Dr B. Whyte (Editorial Office, European Journal of Biochemistry, Postfach, Appolostrasse 2, CH-8032 Zürich, Switzerland) has been appointed Secretary of the IUBMB-IUPAC Joint Commission on Biochemical Nomenclature, JCBN.

ISO Standards

The following are some of the new international standards announced by the International Organization for Standardization (ISO) in recent issues of *ISO Bulletin*.

New international standards published between 13 July 1995 and 11 August 1995:

TC 42	**Photography**
ISO 5989:1995	Photography—Pre-packaged chemicals for the processing of silver halide based photographic materials—Vocabulary
TC 45	**Rubber and rubber products**
ISO 1403: 1995	Rubber hoses, textile-reinforced, for general-purpose water applications—Specification
ISO 3861: 1995	Rubber hoses for sand and grit blasting—Specification

ISO 6224: 1995	Plastics hoses, textile-reinforced, for general-purpose water applications—Specification
ISO 6916-1: 1995	Flexible cellular polymeric materials—Sponge and expanded Cellular rubber products—Specification—Part 1: Sheeting
ISO 11758: 1995	Rubber and plastics hoses—Exposure to a xenon arc lamp—Determination of changes in colour and appearance
TC 61	**Plastics**
ISO 527-3: 1995	Plastics—Determination of tensile properties—Part 3: Test conditions for films and sheets
ISO 1163-2:	Plastics—Unplasticized poly(vinyl chloride) (PVC-U) moulding and extrusion materials—Part 2: Preparation of test specimens and determination of properties
ISO 4587: 1995	Adhesives—Determination of tensile lap-shear strength of rigid-to-rigid bonded assemblies
ISO 4613-2: 1995	Plastics—Ethylene/vinyl acetate (E/VAC) moulding and extrusion materials—Part 2: Preparation of test specimens and determination of properties
ISO 13445: 1995	Adhesives—Determination of shear strength of adhesive bonds between rigid substrates by the block-shear method
TC 147	**Water quality**
ISO 10705-1: 1995	Water quality—Detection and enumeration of bacteriophages—Part 1: Enumeration of F-specific RNA bacteriophages
ISO 10707: 1994**	Water quality—Evaluation in an aqueous medium of the 'ultimate' aerobic biodegradability of organic compounds—Method by analysis of biochemical oxygen demand (closed bottle test)

New international standards published between 12 August 1995 and 14 September 1995:

TC 37	**Terminology (principles and coordination)**
ISO/TR 12618: 1994**	Computational aids in terminology—Creation and use of terminological databases and text corpora
TC 147	**Water quality**
ISO 10634: 1995	Water quality—Guidance for the preparation and treatment of poorly water-soluble organic compounds for the subsequent evaluation of their biodegradability in and aqueous medium

New international standards published between 15 September 1995 and 12 October 1995:

TC28	**Petroleum products and lubricants**
ISO 4264:1995	Petroleum products—Calculation of cetane index of middle-distillate fuels by the four-variable equation
ISO 11223-1:	Petroleum and liquid petroleum products—Direct static 1995 measurements—Contents of vertical storage tanks—Part 1: Mass measurement by hydrostatic tank gauging
TC 35	**Paints and varnishes**
ISO 787-25:	General methods of test for pigments and extenders—Part 25: 1993** Comparison of the colour, in full shade systems, of white, black and coloured pigments—Colorimetric method
TC 45	**Rubber and rubber products**
ISO 1408:	1995 Rubber—Determination of carbon black content—Pyrolytic and chemical degradation methods
ISO 6810:	1995 Rubber compounding ingredients—Carbon black—Determination of surface area—CTAB adsorption methods
ISO 7269:	1995 Rubber—Determination of free sulfur
ISO 7663:	1995 Halogenated isobutene-–soprene rubber (BIIR and CIIR)—Evaluation procedures

** French version of standard previously published in English only

Full details of these and other ISO standards may be obtained from: ISO Central Secretariat, Case Postal 56, CH-1211 Geneva, Switzerland. Tel.: +41 22 749 01 11; Fax: +41 22 733 34 30.

PAC Review

***Pure and Applied Chemistry* (*PAC*) is the official journal of IUPAC. It publishes the main invited lectures of symposia sponsored by the Union; the recommendations of its Commissions on nomenclature, symbols and units, and technical reports on standardization, recommended procedures, collaborative studies and data compilations. Summaries of the most recent IUPAC recommendations on nomenclature and symbols, and technical reports appearing in *PAC* are published in *Chem. Intl.* in the section Recent Reports. In this section we take a brief look at the symposia and lectures published in recent issues of *PAC*.**

This volume of *Pure and Applied Chemistry* contains the plenary and invited lectures presented at the *Second International Symposium on Macrocyclic Ligands for the Design of New Materials*, 29 August–l September 1994, Buenos Aires, Argentina. This Symposium was arranged by ELARG (European Latin American Research Group). Members of ELARG are academics and industrialists with common interests in developing research strategies and enhancing links between Europe and Latin America.

Dr M. Salomon, Official Representative of IUPAC; Prof. P. W. H. Butterworth, Senior Academic Pro-Vice-Chancellor of the University of Surrey, UK; Prof. F. J. Barrantes, Director of the Institute of Biochemical Research at the National University of the South, Argentina; were among the keynote speakers at the opening of this Symposium.

The Symposium was concerned with different aspects of Macrocyclic Chemistry and related areas. The overall and long-term aim of the meeting was to pro-

mote research developments in this field in Latin America through new ideas, contacts, information and expertise.

Two round tables were organized with the participation of European and Latin American panellists, to whom the organisers are most grateful for maintaining the momentum through the discussion sections:

(i) Academic and Industrial Links between Latin America and Europe in Research

(ii) Educational Links between Europe and Latin America in Teaching.

Twelve plenary lectures were given at this meeting, these included:

Calixcrowns and related molecules

Z. Asfari, S. Wenger and J. Vicens (*E. H. 1. C S., URA 405 du C N. R S., 1,* rue *Blaise Pascal, F-67008 Strasbourg France).* Calixcrowns refer to the family of macropolycyclic or cage-molecules in which the monocyclic structures of calixarenes and crown-ethers are combined through the bridging of phenolic oxygens of a calixarene by polyetherchains. The first member of this family was produced by Alfieri *et al.* who reacted pentaethylene glycol ditosylate with *p-tert*-butylcalix[4]arene, in basic conditions, to produce 1,3-*p-tert*-butylcalix[4]crown–6.

In the 25 years since Pedersen reported the synthesis and metal-cation complexing properties of crown-ethers the number of crown-ether compounds has been continuously increasing. Today, the synthesis of a crown-ether molecule is directed toward a desired application, for example, molecular and enantiomer recognition, asymmetric catalysis, redox-properties, allosteric effect, replication, molecular assembly processes, etc. To create these application-directed-macrocycles, chemists have developed the synthesis of macropolycycles or cage-molecules with molecular frameworks combining simple molecular elements containing pre-existing functions. Since 1991, chemists have developed the synthesis of macropolycycles containing, in their molecular structure, the monocyclic structure of calixarenes and crown-ether elements. This combination drives in proximity the hydrophobic cavity of the calixarenes which is able to include organic substrates and the metal cation complexing sites of the crown ether with potential interactions between them. Chemists have already seen evidence of such cation-substrate contact during a triple inclusion by a calixarene—the crystal structure of the Eu(III) complex of bis-(homooxa)-*p-tert*-butylcalix[4]arene showed the Eu(III) to be coordinated to a DMSO molecule included in the hydrophobic cavity of the calixarene.

Calixcrowns are synthesized by systematic reactions of calix[4]arenes with various ditosylates. Depending on the reaction conditions (nature of the base, structure of the ditosylates, and the stoichiometry of the reactants) products with different topologies were isolated (Fig. 2). Calixcrowns were prepared by one-pot procedure. Depending on the nature of the reactants and on the experimental conditions one can induce the reaction towards the formation of calix-*bis*-crowns, double-calixarenes or double-calixcrowns. Alkali metal complexation ability of the calixcrowns was studied and the selectivity of complexation was observed to depend on the number of oxygens in the polyether chain. This fundamental study found an application in the transport of Cs^+ through SLMs with selectivity $Na^+/Cs^+ \approx 1/45\,000$. There is thus the possibility of using these large macrocyclic molecules as efficient devices for the recovery of Cs from waste waters by solvent extraction processes from solvents containing a large excess of Na.

Calix(aza)crowns and 1,3-calix[4]-*bis*-(aza)-crowns were constructed via the Schiff-base intermediates. The Schiff-base-calixarenes were observed to complex preferentially soft cations probably due to the presence of nitrogen atoms. The best systems were for Pb^{2+} and Eu^{3+} with stability constants—5 log units. Zn^{2+} complexation by a calix(aza)crown was studied showing the receptor to occlude two metals by two distinguishable steps.

Host–guest chemistry in the gas phase and at the gas–solid interface: Fundamental aspects and practical applications

Marco Vincenti[1], Claudio Minerol, Ezio Pelizzettil, Andrea Secchi[2], Enrico Dalcanale[2] ([1]Dipartim. di Chimica Analitica, Universita di Torino, Via Giuria 5, 10125 Torino, Italy and [2]Dipartimento di Chimica Organica e Industriale, Universita di Parma, Viale delle Scienze, 43100 Parma, Italy).

The study of host–guest interactions has recently expanded from solution chemistry to the gas phase, where solvent effects are not present, allowing better understanding of the intrinsic phenomena responsible for molecular recognition. Important aspects

Fig. 1 Dr Angela F. Danil de Namor (University of Surrey) who was one of the organizers of the *Second International Symposium on Macrocyclic Ligands for the Design of New Materials* in Buenos Aires.

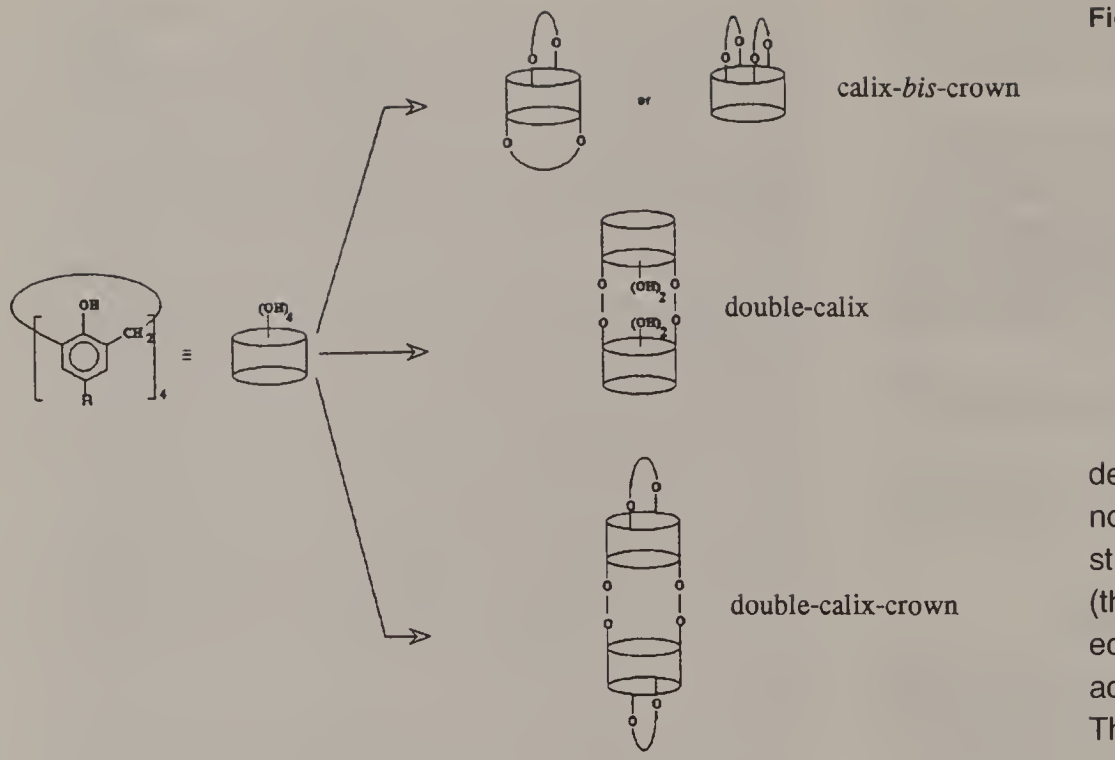
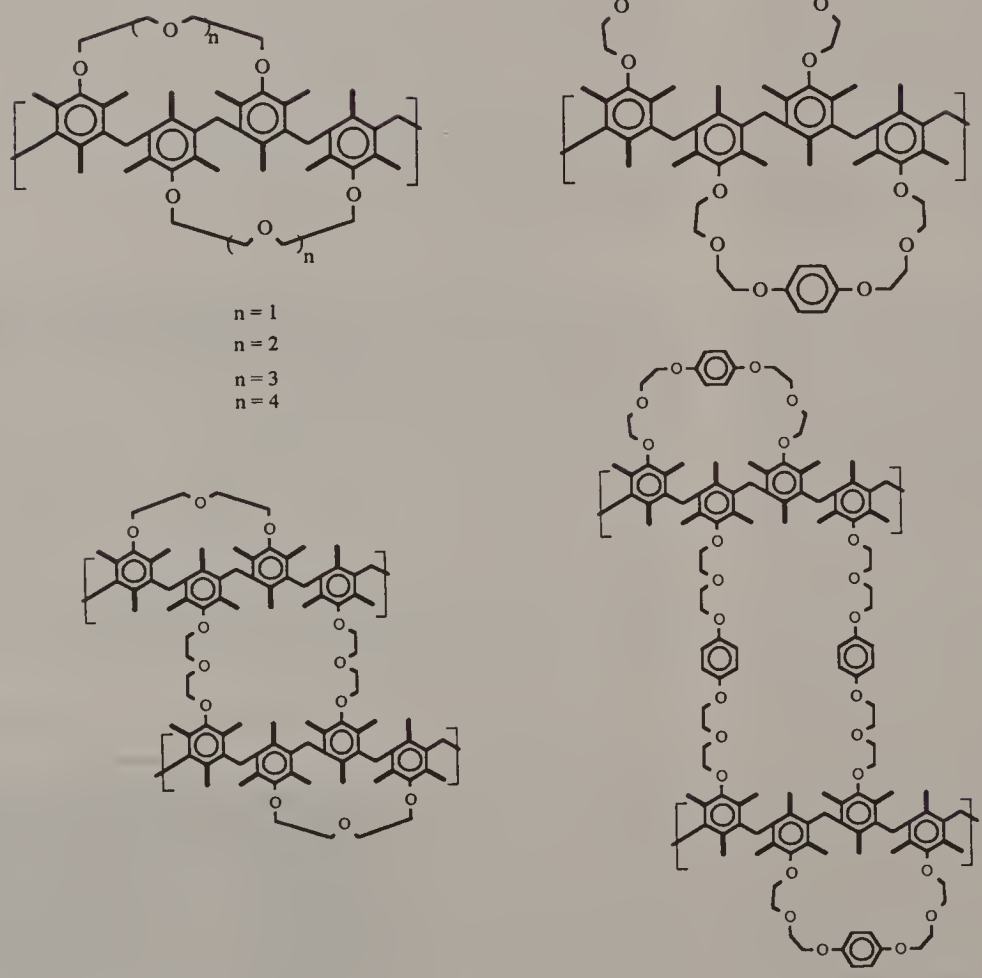


Fig. 2 Different pathways to calixcrowns.



under investigation include the mechanism of interaction, the identification of binding groups, as well as the discovery of structural requirements for the host to undergo inclusion complexation. The information gained from these gas phase studies can be exploited to design new practical applications of host–guest chemistry, particularly when gas–solid interactions are involved. Analytical devices such as gas-sensors and chromatographic adsorbing cartridges take advantage of the structural recognition capability of the host to achieve high levels of selectivity.

The term 'host–guest chemistry' is generally used to designate the establishing of multiple noncovalent bonds between a large and structurally concave organic molecule (the host) and one or more simple molecules or ions (the guest), which will be accommodated inside the host cavity. The excellent skills of many groups of organic chemists has resulted in the production of a large variety of synthetic hosts with different size, geometry, binding sites, portals and chemical and physical properties. This tremendous effort in synthetic chemistry has developed the need for some simple methods that could predict which structural features of the host are necessary to achieve high complexation constants and high selectivity toward a definite class of guests. Among these methods, the present authors have proposed to study the gas phase properties, as the absence of solvent effects could result in better comprehension of the fundamental aspects responsible for supramolecular interactions.

In previous studies, we formed gaseous host–guest complexes in high yield, by rapid vaporization of the host within a mass spectrometer ion-source, filled with a mixture of a buffer gas (methane) and one or more gaseous guests present in known relative concentration. Once formed, host–guest complexes were mass-analyzed and detected as positive and negative ions. A series of conclusions were drawn from previous studies involving cavitands 4-T_2 and 3-T_2 (Fig. 4), are listed below:

(i) the formation and relative abundance of host–

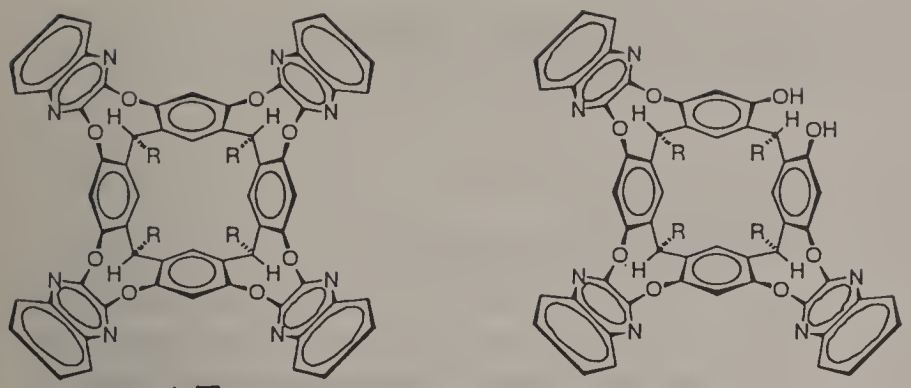


Fig. 3 Cavitants.

guest complexes do not depend (or has little dependence) on their charge polarity, *viz.* the results obtained from positive and negative ions mass spectra were very similar;

(ii) the predominant process in gas-phase inclusion complexation is the interaction between the charged host and the neutral guests, but a neutral-neutral interaction mechanism may occur to some extent;

(iii) the complexation of aromatic guests is driven by CH–π interactions;

(iv) the extent of complexation strongly depends on the chamber temperature;

(v) the reacting system reaches a condition of thermodynamic equilibrium;

(vi) consequently, when mixtures of candidate guests are present in the gaseous atmosphere, their relative complexation constants can be determined.

All together, these observations constitute the basis for a new methodology, directed to the investigation of the fundamental aspects of host–guest complexation. For example, it was demonstrated that 4-T_2 has high selectivity toward aromatic guests, provided that multiple CH–π interactions could be established between the host and the guest (i.e. pentafluorobenzene does not form complexes). On the other hand, cavitand 3-T_2 was able to form extremely stable inclusion complexes only with those guests that could establish a hydrogen bond with its phenolic hydroxyls and, at the same time, CH–π interactions on the aromatic rings of the opposite quinoxaline.

While a variety of guests have been tested, observations concerning the role of the host and the requisites for it to undergo inclusion complexation were restricted to cavitands 4-T_2 and 3-T_2. A more general perspective on the structural features needed by the host to form stable host–guest complexes in the gas phase is necessary. The present research is intended to provide a contribution to this work by comparing the gas phase interactions established between a few selected mixtures of guests and a series of eight bridged calixarenes with a common basic substructure (that of calix[4]arene) and various bridging units, with different length, rigidity and functional groups.

Gas-phase experiments were performed using a Finnigan-MAT hybrid tandem mass spectrometer, with magnetic, electrostatic and quadrupole analysers mounted consecutively. Host–guest complexations were run in the ion-source of the mass spectrometer and the reaction products were detected at the first electron multiplier, located after the electrostatic sector. The ion-source volume was the one typically used for chemical ionization experiments. It was preliminarily filled with a gas mixture composed of small amounts of two competing candidate guests (about 0.5% each) and a large excess of methane (99%). The excess of methane provided constant conditions of thermostatisation of the reacting system and ionization of the reaction products, independently from the specific candidate guests used in each experiment The relative partial pressure of the two guests was determined by headspace gas chromatography. Relative and total (30 Pa) pressures were adjusted using regulating valves. The ion-source was kept at 50 °C. When a stable composition of the ion-source atmosphere was reached (it took about 30 min), a small amount (i.e. 30–50 ng) of the candidate host was introduced in it by fast vaporization from a DCI wire, where it had been deposited as a thin film of molecular layers. Once in the gas-phase, the excess of thermal energy was removed from the host by multiple collisions with methane molecules, and then the host could interact with the candidate guests to produce inclusion complexes, under thermodynamically controlled conditions. The reaction products were determined both as cations and anions.

It was thought that the knowledge gained from our gas-phase studies could be exploited in some analytical applications, involving the occurrence of host–guest interactions at the solid–gas interface. Although these interactions are possibly different in many respect from those occurring in the gas-phase, both situations are characterized by the absence of any solvent, that usually plays an important role in solution host–guest chemistry. Consequently we experimented by placing the cavitants on a neutral solid support and using this modified solid as a separation medium in chromatography. The preliminary results obtained by using supported cavitands 4-T_2 and 3-T_2 as the adsorbing materials for volatile analytes in a purge-and-trap device were encouraging.

Commission and Committee News

Summary Minutes from the meeting of the IUPAC Commission on Molecular Structure and Spectroscopy (I.5) at the IUPAC General Assembly in Guildford, 5–7 August 1995

Emphasis on theoretical chemistry

Together with a variety of IUPAC standing committees, division committees and numerous commissions, subcommissions and working parties, the Commission on Molecular Structure and Spectroscopy (I.5) met in Guildford on a warm Summer weekend from 5th to the 7th of August 1995. This Commission of 11 members was initiated in 1955 and can therefore celebrate 40 years of activity. The status of various current projects was reviewed, progress reports were evaluated and plans for new potential projects within the fields of molecular structure and spectroscopy were discussed.

The subcommittee on Infrared and Raman Spectroscopy, chaired by Professor James R. Durig (Chairman of Commission I.5 1983–1989) was terminated after a long tenure and many completed projects. Prof. Durig's work for the subcommittee and for the Commission, which he chaired for several years, was recognized and appreciated.

In order to emphasize the increasing importance of numerical quantum chemical calculations, which are increasingly used as a consequence of ever cheaper computer time and access to widespread programs, a new subcommittee on Theoretical Chemistry was established with Prof. James E. Boggs as chairman. Commission I.5 also voted to support an eventual change of name of the Physical Chemistry Division to the Physical and Theoretical Chemistry Division, in order to stress the increasing importance of theoretical chemistry.

Wavenumber calibration standards for infrared spectroscopy, essential to all spectroscopists, were first published by IUPAC in 1961. They were extended and revised in 1973 and in 1978. Much later, the development of standards for intensity measurements in infrared spectroscopy was initiated, and this work was brought to a happy conclusion with the publication of the book: *Tables of Intensities for the Calibration of Infrared Spectroscopic Measurements in the Liquid Phase,* by J. E. Bertie, C. D. Keefe and R. N. Jones, Blackwell Science, 1995 (IUPAC Data Series no. 40—see *Chemistry International* 1995, **17**(4), 139). The standards are based upon experimental infrared bands of benzene, toluene, chlorobenzene and dichloromethane measured with Fourier transform spectrometers. A program IRYTRUE was developed and is supplied on a diskette with the book, as are the standard bands. Prof. John E. Bertie is the present chairman of Commission I.5 while Dr R. Norman Jones was secretary of this Commission from its founding in 1955 and was later president of the Physical Chemistry Division (1975–1977). This volume is therefore a 40th birthday present to Commission I.5 from one of its founding members.

Two additional projects: *Symbols for Fine and Hyperfine Structure Constants and Notations,* led by Eizi Hirota, and *Guidelines on Nuclear Magnetic Resonance Computerized Databases,* led by Charles Wilkins, have been published in *Pure and Applied Chemistry* in the past biennium. The papers, *Conventions in Molecular Spectroscopy (part I-3)* are in the final correction stage and will be reported in *PAC* in the near future.

Three projects were terminated since no progress had been made since the Lisbon meeting, while four projects were continued. One of these is an ambitious project to be published as the book: *Non-linear Spectroscopy for Molecular Structure Determination,* editor S. Tsuchiya, with chapters by an international group of contributors.

Five new projects were proposed and were subsequently approved by the Physical Chemistry Division. Their titles and leaders are: *Spectroscopic Intensities; Related Quantities. Nomenclature and Symbols* (J.E. Bertie); *Spectroscopy under Extreme Conditions of Pressure and Temperature* (A. M. Heyns); *Parameters and Symbols for Nuclear Magnetic Resonance Spectroscopy* (R. K. Harris); *The Computation of Experimental Structure and Properties of Small Molecules by ab initio Calculations* (R. Janoschek) and *Guidelines for Presentation of Methodological Choices in Computational Chemistry* (J. E. Boggs). The two latter projects will be carried out within the new subcommittee on Theoretical Chemistry.

Commission I.5 had constructive discussions of topics of mutual interest with Commissions V.4 (Commission on Spectrochemical and other Optical Procedures for Analysis), I.3 (Commission on Electrochemistry) and I.1 (Commission on Physicochemical Symbols, Terminology and Units). These discussions gave good ideas to both parties, led to collaborations on existing projects, and helped to avoid overlap in projects of different commissions.

The next full meeting of the Commission is planned at

the 39th General Assembly in Geneva in 1997, while the working groups for new and continuing projects may convene in 1996, possibly at an international conference.

Peter Klaeboe
(Secretary Commission I.5)

Summary Minutes of the meeting of the IUPAC Commission on Atomic Weights and Isotopic Abundances (II.1), Guildford, UK, 5–7 August 1995

Atomic Weights

Twenty-three members of the Commission on Atomic Weights and Isotopic Abundances (II.1), including national representatives and observers, met for three days during the 38th IUPAC General Assembly in Guildford, UK. Four new members were elected to the Commission.

The Commission has revised its table of atomic weights. The atomic weights of five elements have been changed significantly. Based on new determinations of isotopic abundances and reviews of previous isotopic abundances, the atomic weight of boron was changed from 10.811(5) to 10.811(7), of carbon from 12.011(1) to 12.0107(8), of cerium from 140.115(4) to 140.116(1), of europium from 151.965(9) to 151.964(1), and of platinum from 195.08(3) to 195.078(2). These new data are a significant improvement on the previous values which were based on determinations between 1947 and 1969.

In light of new atomic mass data, the Commission has recommended small changes to the atomic weight of the following monoisotopic elements: sodium, aluminum, phosphorus, manganese, cobalt, arsenic, caesium and bismuth. The Commission recommended changes to the uncertainty values of the following monoisotopic elements: fluorine, scandium, rhodium, praseodymium, terbium, holmium, thulium and gold.

The Commission has noted that relative lithium isotopic ratios are being expressed both as $^{7}Li/^{6}Li$ ratios and as $^{6}Li/^{7}Li$ ratios, leading to confusion. The Commission has recommended that $^{7}Li/^{6}Li$ ratios be expressed relative to L-SVEC lithium carbonate and that reporting of $^{6}Li/^{7}Li$ ratios be discontinued.

It has come to the attention of the Commission that the $^{37}Cl/^{35}Cl$ ratio of ocean water is not constant. Therefore, the Commission has recommended that relative chlorine isotopic ratios be reported relative to the isotopic reference material NIST SRM 975 sodium chloride, and that reporting chlorine isotopic ratios relative to SMOC (Standard Mean Ocean Chloride) be discontinued.

The Commission has noted that the reference material used for several decades for reporting relative sulphur isotopic ratios is inhomogeneous. Therefore, the Commission has recommended that relative sulfur isotopic ratios of all substances be expressed relative to VCDT (Vienna Canon Diablo Troilite) on a scale such that the $^{34}S/^{32}S$ of IAEA-S-1 silver sulfide is 0.9997 times that of VCDT. The Commission recommends that reporting of sulphur isotopic ratios relative to CDT be discontinued.

The Commission has noted comments on the Internet that were critical of Commission recommendations from the 37th General Assembly in Lisbon concern expressing hydrogen, carbon, and oxygen isotopic results relative to VSMOW (Vienna Standard Mean Ocean Water) or VPDB (Vienna Peedee Belemnite). The Commission reaffirms it recommendation that $^{18}O/^{16}O$ ratios of all substances be expressed relative to either VSMOW or VPDB on scales such that the $^{18}O/^{16}O$ of SLAP (Standard Light Antarctic Precipitation) is 0.9445 times that of VSMOW. For oxygen-isotope ratios, in the event that one is not able to calibrate to the VSMOW-SLAP scale, one should indicate the isotopic composition obtained relative to VSMOW or VPDB for a reference material of the same material or compound.

Immediately prior to the Lisbon General Assembly, the Commission's Subcommittee for Isotopic Abundance Measurements, Subcommittee on Natural Isotopic Fractionation, and Subcommittee on Non-Terrestrial Isotopic Abundance Data met at the Institute of Reference Materials and Measurements of the Commission of the European Communities Joint Research Center in Geel, Belgium on 31 July and 1 August 1995.

The chairman of the Subcommittee for Isotopic Abundance Measurements, Prof. Kevin J. R. Rosman from the Curtin University of Technology in Perth, Australia, reported that new isotopic data on 18 elements lead the Subcommittee to recommend revision of the atomic weights of boron, carbon, europium, cerium, and platinum, and to recommend changes to the Table of the Isotopic Composition of the Elements for boron, carbon, silicon, krypton, xenon, cerium, europium and platinum.

The chairman of the Subcommittee for Natural Isotopic Fractionation, Prof. H. Roy Krouse from The University of Calgary in Calgary, Canada, gave a detailed report on 13 chemical elements that show variation in isotopic composition in naturally occurring terrestrial materials, and thus, variation in their atomic weight. Extensive graphical presentation of these data was presented in a report that is planned for publication in 1996.

The Subcommittee for Non-Terrestrial Isotopic Abundance Data continued its literature evaluation under the leadership of Prof. Ludolf Schultz from the Max-Planck-Institut für Chemie. Data in this area is expanding at a great rate, and the Subcommittee's review of hundreds of articles forms the base of a report that

will be published as part of the 'Atomic Weights of the Elements 1995.'

An archive for Commission II.1 documents has been established at the Chemical Heritage Foundation, Philadelphia, PA, USA. Dr Tyler B. Coplen, Dr H. Steffen Peiser, and Mr Thomas Murphy, reported that they have worked to acquire and organize documents dating from 1827 in this valuable Commission asset.

The next meeting will be held in Geneva, Switzerland, August 1997 during the 39th General Assembly.

Dr Tyler B. Coplen
(Secretary Commission II.1)

Summary minutes of the meeting of the IUPAC Commission on High Temperature and Solid State Chemistry (II.3), Guildford, UK, 5–7 August 1995

During the past biennium, Commission II.3 has continued to work partly in classical IUPAC nomenclature and standardization areas while also undertaking projects useful to the international chemical community which can be completed on shorter time scales. The result has been a rationalization of the Commission's activities.

Three publications have appeared in *Pure and Applied Chemistry*: **Nomenclature of Graphite Intercalation Compounds**, which will also will be a chapter in Red Book 2; **Definition of Terms Relating to Phase Transitions of the Solid State**; and **Recommended Terminology for the Description of Carbon as a Solid.** The latter is the result of the work over a number of years of the subcommittee for carbon terminology and contains some 121 terms.

Articles describing an IUPAC collaborative study on **The Electrical Conductivity of Cubic Stabilized Zirconia** are in press in *PAC* and *Solid State Ionics*.

The Commission has also compiled and distributed on request, A selection of textbooks and reference literature, in English, on Solid State Chemistry and Related Areas. This was publicized through an article on the teaching of solid state chemistry in *Chemistry International* and through the *CTC Newsletter*. A follow-up project will describe a number of laboratory experiments suitable for the teaching of solid state chemistry at University.

The Commission continued its highly successful series of Conferences on High Temperature Materials Chemistry.

HTMC VIII was hosted by Profs. Komarek and Mikula in Vienna in April 1994 and was attended by more than 160 delegates. These meetings are made possible by the international composition and unique mix of expertise of the Commission. HTMC IX will be held at Pennsylvania State University, PA, USA, 19–23 May 1997.

At Guildford the Commission approved two further manuscripts for publication subject to satisfactory review. These are **Quantitative Analysis of a PbO–SiO_2 glass by Election Microprobe** and **Characterization of SiC Powders and the Influence of Powder Properties on Sintering**. The Commission also reviewed a draft manuscript on **Terminology for Diffusion in the Solid State** and recommended further consultation with relevant experts prior to publication.

The Commission approved a programme plan for the Joint Project with the Macromolecular Division on sol-gel and polymer-derived ceramics, glasses and ormocers. Initial meetings of project participants took place during the Guildford General Assembly.

The Commission, after consideration of reports from Preliminary Survey Teams, selected four projects for its future work programme. In addition, the Commission will continue preparation of a bibliography designed to assist in the inclusion of material on high temperature chemistry in university chemistry courses. Subcommittee 2 of the Commission also reported progress at Guildford; the Subcommittee will prepare an up-to-date summary and assessment of national procedures used for the Characterization of Carbonaceous Materials and New Carbons.

Considering the future, the Commission was mindful that, in line with the objectives and needs of IUPAC's National Adhering Organizations, IUPAC should promote chemistry and advance its usefulness to the worldwide community. To do so, the Union, in addition to programmes in nomenclature and standardization, should carry out selected programmes in areas in which chemistry has a key role to play in the service of mankind. One of these areas is chemistry as applied to materials and this is the area in which the work programme of Commission II.3 is focused. The expertise of the Commission lies in the preparation, study and characterization of inorganic materials and of high temperature systems. To reflect its programmes and objectives the Commission requests that its name be modified to The Commission for High Temperature Materials and Solid State Chemistry.

The next meeting will be held in Grenoble, France, 14–15 June 1996. The Commission will also meet informally at Penn State on 24 May 1997, immediately following HTMC IX, before the 39th General Assembly in Geneva.

Dr Gerd M. Rosenblatt
(Secretary, Commission II.3)

Summary Minutes of the meeting of the IUPAC Commission on Nomenclature of Organic Chemistry (III.1)

The 1995 meeting focused mainly on the P-names project. This project is concerned with selecting a set of rules to generate a single name for each organic com-

Members of Commission II.1

pound, a name to be used in legal situations such as international commerce. At present these names are referred to within CNOC as *preferred names,* but this designation may be changed. P-names are based on *substitutive* nomenclature. Discussions of draft documents highlighted the need for firm, clear choices among IUPAC-approved alternatives, and substantial progress was achieved by firm choices in four areas.

(a) **Priority among rings and chains:** Assembles with at least three rings connected by chains will be named by phane nomenclature. For others, a set of criteria based on the number of skeletal atoms (in the ring or the chain), number of substituents, and seniority of rings was accepted to determine ring vs. chain priority. The concept of centrality, suggested at the previous meeting, was abandoned.

(b) **State of hydrogenation:** For P-names, CNOC decided that the state of hydrogenation of a parent hydride will be expressed as a prefix (hydro/dehydro) or an ending (ene/yne) adjacent to the parent hydride stem. These prefixes and endings will have parallel status so far as numbering is concerned, and the prefixes are not included in the alphabetizing of substituent prefixes.

Examples: 3-methylcyclohex-1-ene, 7-methyl-1,2-dihydronaphthalene; cyclohex-2-en-1-ol, 7,8-dihydro-2-naphthol.

(c) **Acyl groups:** Infix nomenclature will be used for acid groups in which oxygen has been replaced by a hetero atom. For example: phosphorothioyl *(not* thiophosphoryl), and sulphonothioyl *(not* thiosulphonyl). (A few traditional names are to be retained: e.g. thioacetic acid. For P-names, the discussion favoured elimination of most retained names.)

When a carbonyl-containing group (such as ester) can be counted as part of a parent chain, but not as the principal group, it is included in the parent chain; i.e., the group is not named as a substituent. *Example:* 5-methoxy-5-oxopentanoic acid *(not* 4-(methoxycarbonyl)butanoic acid]. If an acyl group related to a monobasic acid is not part of the parent chain and must be treated as a substituent, use the acyl name, except for – COOH, for which carboxy is retained.

(d) **Amines**; For the P-name project, a clear choice between azane parent and an alkane parent with amine suffix was required. Although a strong case was made by some persons for azane as parent [e.g. (2-methylbutyl)azane], a small majority favored the use of the larger parent and amine suffix (2-methylbutan-1-amine). Radicals and ions centered on N will be named systematically by use of suffix modification of -amine: -aminyl, -aminium (not ammonium), -aminide. The documents under consideration will be revised on this basis.

The need for a standard symbolism for free valence in formulas became apparent, and CNOC agreed to recommend adoption of a wavy line perpendicular to the bond line(s) for the free valence(s): ——≷.

A document on spiro compounds is nearly ready to be sent to referees. The final version of **Basic Terminology of Stereochemistry** is to be submitted in September for publication. A draft of a recommendation on fullerene nomenclature will be sent to principal workers in the field for review and comments, possibly by the end of this year. The document on natural products needs only minor editing and is to be sent to IDCNS in September. The **Glossary of Class Names of Organic Compounds and Reactive Intermediates Based on Structure**, a joint project of the Commissions on Nomenclature of Organic Chemistry and Physical Organic Chemistry, was published in the Aug/Sept 1995 issue of *Pure and Appl. Chem.* A World Wide Web version of this document, prepared by Dr G. P. Moss (a CNOC participant), is available.

The next meeting will be held in Prague, Czech Republic, 15–19 August 1996 (arrival 14 August).

Prof. James G. Traynham
(Secretary of Commission III.1)

Summary minutes of the meeting of the IUPAC Commission on Equilibrium Data (V.6)

The Commission launched the second release of the Stability Constants Database, SC-database (IUPAC/ Academic Software). The occasion was marked by the attendance of Alan McNaught (Manager, Journals, R.S.C.) and a small ration of French Champagne! This release includes the four earlier book volumes published by the Chemical Society (London) and IUPAC and establishes a complete coverage of the literature from 1890 to 1993.

The SC-database is seen as a valuable resource for further Commission activities. We propose the preparation of teaching material for solution equilibria. This will be in the form of a series of tutorials covering both fundamental and applied aspects of solution equilibria. The tutorials will be multimedia, involving written text, computer simulation and use of a small database derived from SC-database. An important element of the programme will be testing of the material in class room situations in both developed and developing countries. Other developments with SC-database will be the introduction of evaluations to flag 'Recommended Values' and enhancement of speciation and other software packages.

A major policy decision concerned the format for future 'Critical Reviews of Stability Constants'. The criteria for 'recommended values' (M. T. Beck, *Coord. Chem. Rev.* 1975, **17**, 358–359) will not change, but future Reviews will not include discussions substantiating other classifications or the rejection of data. The result will be a more concise article, simply identifying the most reliable or 'recommended values'.

V.6. is experiencing good collaboration with other Commissions in the Analytical Division. A joint working party with V.8. has commenced work on the **Thermodynamics of the solubility and solution equilibrium reactions of metal-macro-cyclic complexes** with a view to project initiation in 1996. A new project on **Influence of pressure on chemical equilibria in aqueous solutions, with particular reference to sea water** has the support of V.9. through liaison between Prof. David Turner (V.9.) and Prof. Robert Byrne (V.6.). A new project titled **A review and critical analysis of equilibrium and redox data for porphyrins and metalloporphyrins** (coordinators Masaaki Tabata (V.6.) and Karl Kadish (V.5.)) also brings together the interests of two Commissions.

The next meeting will be held in Budapest, August 1996.

Dr Kip Powell
(Secretary of Commission V.6)

Summary minutes of the meeting of the IUPAC Commission on Food Chemistry

The Food Chemistry Commission of the Applied Chemistry Division met in Guildford (UK) during the General Assembly, to consider its future orientation and priorities. Besides the review of current projects suggestions for initiating new projects were considered—especially in the following areas:

1. Training and Technology Transfer

Future projects will focus on training in analytical methodology and quality assurance by organizing workshops and symposia. Priority will he given to workshops organized in collaboration with United Nations Agencies for young scientists from less developed countries. These workshops will aim at capacity building and sustainable development of monitoring programmes in food and environmental studies.

This new orientation is already being implemented with two workshops sponsored by UNESCO which were held in November 1995: one in the Dominican Republic on Ciguatera and a second in Tunisia on Ochratoxin. Next year in Rome, a workshop on **Practical Considerations of Food Analysis For Mycotoxins and Phycotoxins** will be organized in collaboration with FAO in conjunction with the Ninth International IUPAC Symposium on Mycotoxins and Phycotoxins.

To develop this new orientation, the membership of the Commission has been adjusted to give a better geographic distribution of Members. This will be important in the potential organization of future workshops in some specific regions such as Southern America and Eastern Europe.

2. Nutrition and Disease Prevention

Future projects will focus on positive aspects of diet and health. Proposals are being developed for the initiation of work on evaluation of risk/benefit ratio in particular foods. Also, future project proposals are being considered on the role of food constituents in human health protection, e.g. in disease resistance and cancer prevention.

The Commission decided to reinforce connections to other International Organizations such as Codex Alimentarius, especially the Codex Committees on Methods of Analysis and Sampling, and on Food Additives and Contaminants.

The Commission will meet next in Rome at the Ninth International IUPAC Symposium on Mycotoxins and Phycotoxins.

J.Marc Fremy and David McWeeny
(Commission V.6)

Ultrafast chemistry with lasers

One of the early uses of the laser by chemists was as a source of monochromatic light. With time, however, additional uses of the laser were discovered, for example, when tuneable lasers became routinely available, the field of molecular spectroscopy was revolutionised. As lasers increased in sophistication and reliability, it became possible to measure a molecular transition with ever increasing precision. Indeed, the point arrived when the field of ultra-high-resolution molecular spectroscopy was born, the routine measurement of linewidths to an accuracy of better than 1 in 10^8.

However, not only is the ability of controlling the wavelength of a laser pulse changing chemistry, it is now also possible to obtain variability in the pulse duration. Indeed, it is now routinely possible to generate laser pulses which are only a few fringes of light in length. Consider a 25 femtosecond pulse at a wavelength of 600 nm; that is, one such pulse has a spatial extent of $25 \times 10^{-15} \cdot 3 \times 10^8$ (speed of light) $= 75 \times 10^{-7}$ m, which with $\lambda = 600 \times 10^{-9}$ m gives a pulse of either 12 or 13 fringes of light at this wavelength. It is the uncertainty principle which will limit our ability to produce very much shorter laser pulses—if you have fewer fringes then you are forcing the photon to be increasingly localised—thereby seeking to violate Heisenberg's principle.

In most small molecules there is likely only to be one chromophore, that is, the part of the molecule, perhaps a bond where the oscillating electric dipole moment is

Wavepackets

It is from a consideration of the localization of the photon in a narrow time frame that many interesting properties of ultrashort laser pulses are derived. Consider a time dependent phase factor for a wavefunction of definite energy. The wavefunction, for a particle of mass m moving in the x direction, e^{ikx}, corresponds to an energy $E = k^2h^2/8\pi^2m$, where k is the wavevector. Thus, we may write the full time-dependent wavefunction

$$\Psi_k(x,t) = Ae^{ikx}\ e^{-i2\pi Et/h} = Ae^{ikx - ik2ht/4\pi m},$$

The particle under consideration was, of course, prepared with an imprecise energy. Since the energy is imprecise the wavefunction has to be a superposition of wavefunctions, each one corresponding to a different energy. That is, we form a wavepacket. Since k is a continuously variable parameter the sum is really an integral over k, and so the wavepacket is

$$\Psi = \int g(k)\, \Psi_k(x,t)\, dk,$$

Due to interference between the phase factors, at one instant the overall wavefunction will have large amplitude at one point, however, this point will change in time due to the time dependence of the destructive interference. This implies that the location of even a static particle spreads with time.

What this implies for a femtosecond pulse is that a pulse of, for example, 30 fs duration must consist of a set of frequencies spanning a halfwidth of 300 cm^{-1}. Consequently, as the pulse gets shorter, the wider the spread of frequencies—it is impossible to have a monochromatic ultrashort pulse. Thus the short pulses used to probe molecules do not, in general, excite single rotation-vibrational levels.

Such a short pulse will excite molecules from a ground state to some excited state, because of the lack of monochromisity many vibrational states will be populated in the upper state. However, these individual waves interfere to give a state which is localized, as opposed to spread over the whole of the upper state potential. This superposition of vibronic states is the wavepacket and because it is coherent it is amenable to detailed mathematical analysis—its evolution on the upper electronic surface can be followed.

This is the important difference between the excited state prepared by a femtosecond and a continuous wave laser source. In the latter case, the component vibronic states have no fixed phase relationship to each other and the sum of their spatial distributions does not change with time. The excited state is spatially delocalized. The continuous wave source creates a series of wavepackets on the upper surface which are smeared out.

able to come into resonance with incident radiation, which is actually absorbing the laser radiation. The observation that energy, of order, a visible photon (a couple of electron volts) could be selectively placed in one particular bond in a molecule initially lead to the idea of bond-selective chemistry. That is, that activation of one bond, might under appropriate conditions lead to increased chemical activity of that bond. For example, if the absorbing molecule was involved in a chemical reaction involving a bond breaking process, if sufficient energy could be put into one part of the molecule, perhaps that part nearest the centre of bond fissuring, then the reaction rate might be influenced by the presence of the laser light.

Unfortunately, early expectations of developing bond selective photochemistry soon gave way to disappointment. As lasers developed, it became possible to produce shorter and shorter laser pulses. Pulses whose duration are shorter than the rate at which energy moves from one bond to another bond within a molecule. Such photochemical studies with short pulses of laser light clearly showed that even though one bond might initially absorb a photon, this energy was redistributed within the other bonds of the molecule on a time scale fast when compared to the rate of the various chemical reactions. Consequently, there was no bond-selective effect of laser light on chemical reactions. The energy was deposited into a particular bond, however, it was coupled to other bonds in the same molecule through a densely packed vibrational density of states and by absorbing short laser pulses one was doing little more than heating the molecule. Such initial disappointments do not, of course, deter everybody. Indeed, they can act as a spur for further investigation and have allowed us to understand a great deal of new physics concerning vibrational interactions in molecules. The goal of being able to use precisely tuned laser light to control the outcome of a chemical reaction is too seductive to be ignored for long. Indeed, the idea of using a laser like a molecular-scale scalpel was so seductive that the magazine *Fortune* ran a story in 1977 entitled 'Laser Alchemy is Just Around the Corner'. It said chemists would soon be fashioning new fuel, drug molecules and detergents at will.

An excellent review of the current status of the application of ultrafast laser technology to study basic, indeed, very old problems in chemistry has recently been published. *Ultrafast Processes in Chemistry and Photobiology*, eds M. A. El-Sayed, I. Tanaka and Y. Molin, has been published as part of the *Chemistry for the 21st Century* series of monographs by IUPAC. Some notable chapters include:

Femtochemistry (Chapter 1, Prof. A.H. Zewail, Arthur Amos Noyes Laboratory of Chemical Physics, California Institute of Technology, Pasadena, USA)
In all classes of elementary chemical reactions, bond making and bond breaking, one is involved with nonequilibrium species. These structures are commonly called reaction intermediates or activated complexes and denoted, for example, as

$$A + BC \rightarrow [A..B..C]^* \rightarrow AC + B,$$

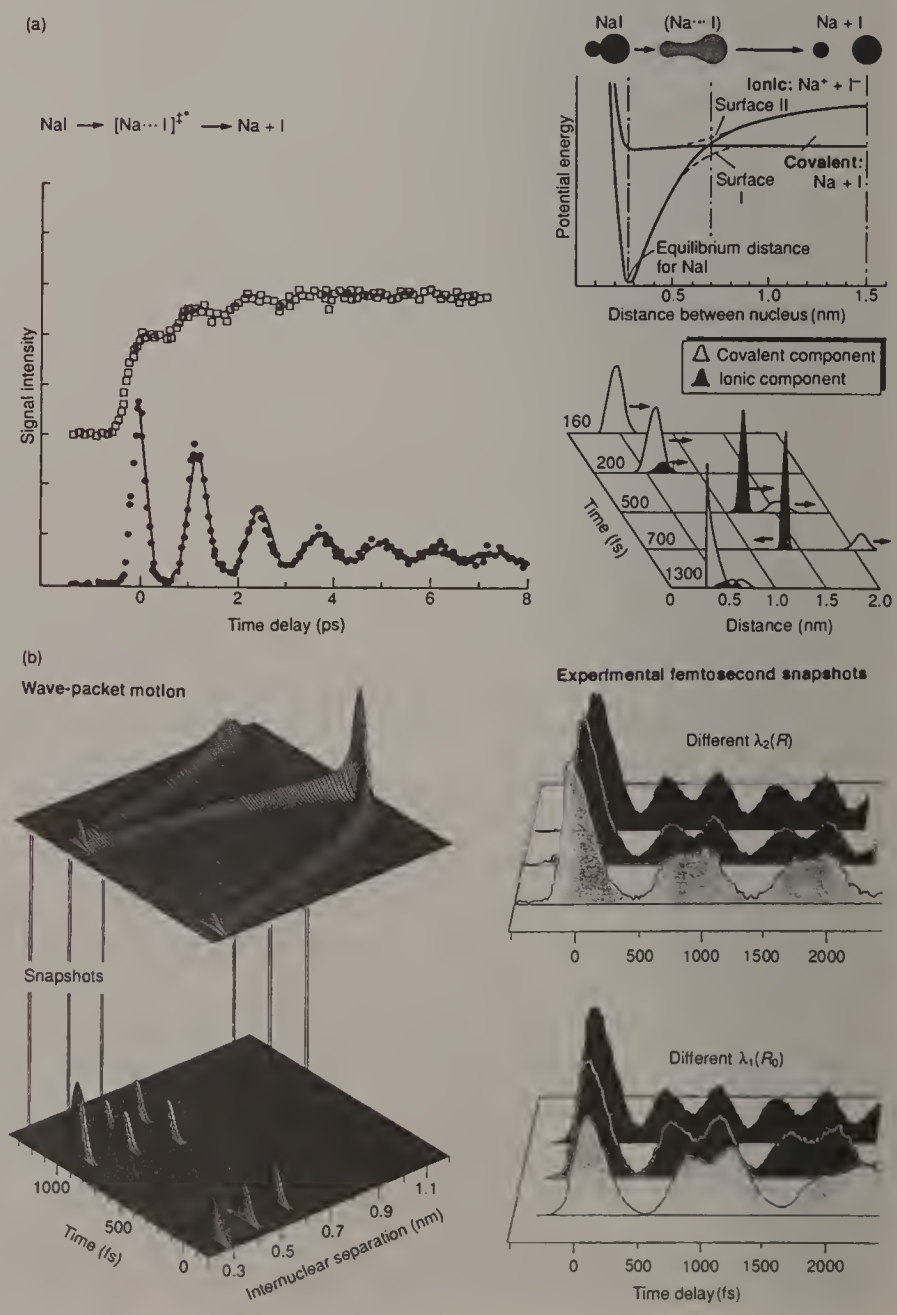


Fig. 1 (a) Femtosecond dynamics of the NaI reaction. (Left) The experimental observation made by detecting the activated complex [Na..I]* (circles) and the free Na atom (squares). (Right) The covalent and ionic potentials and the quantum mechanical calculations of the wave-packet motion. (b) The trajectories in real time, theoretical (left) and experimental (right). Shown in the experimental transients are the first three peaks of the resonance in (a), but now split indicating the motion of the wave-packet in and out of the probe (λ_2) window. λ_1 is the pump wavelength.

The idea of such a transition state in chemical reactions goes back to 1931 and has been the basis of much of our theories of chemical reaction dynamics.

The passage from reactants to products, with a continuous change in nuclear separation and geometry, is very rapid, £ 1000 fs. Consequently, it is only with the development of ultrashort laser pulses that it has been possible to probe the dynamics and structure, spectroscopically, of these reaction intermediates during a chemical change. The essence of femtosecond transition-state spectroscopy (FTS) involves an initial femtosecond pulse which sets the zero of time for the reaction and synchronises all reactant molecules in a particular nuclear configuration. The subsequent probing pulse views the system either in the transition state or at separations corresponding to different configurations, including the asymptotic product state. A surface of measurements, $I(t,\lambda)$, provides the nature of the dynamics: for a given wavelength ($I_{infinite}$ for final products, or I^*_1 I^*_2...etc. for transition states), the time scan, (t) gives the femtosecond transient $I(t,\lambda)$ for probing at $R_{infinite}$ or at R^*_1, R^*_2...etc. The duration of the pulses is generally shorter than the lifetime of the transition state, and this allows the monitoring of the transient structure with $\approx 10^6$-fold increase in sensitivity when compared with continuous wave (CW) laser or nanosecond (which is essentially the same thing for a femtosecond phenomenon) techniques.

Consider the alkali halide reactions, for example,

$$NaI^* \rightarrow [Na...I]^* \rightarrow Na + I.$$

The potential energy surfaces for such a reaction is well described by the covalent (Na + I) and ionic ($Na^+ + I^-$) curves, which cross at a certain internuclear distance (see Fig. 1).

As the wave-packet, prepared at time zero, moves from the covalent to the ionic curve, the chemical bond will also change in character from being purely covalent to ionic. It was Linus Pauling who pointed out that the crossing or mixing of covalent and ionic potentials was a means of characterising chemical bonds. When the reaction intermediate was probed spectroscopically in the region of the transition complex, a resonance motion between the covalent and ionic curves, with a damping determined by the leakage probability through the resonance, was observed. However, when free Na atoms were observed, an increase in the number of sodium atoms was observed each time the system executed a resonance, that is, a series of quantized steps determined by the period of covalent to ionic motion, was observed. Such observations, see Fig. 1, have been related to the resonance period, the lifetime of the activated complex, the escape probability and the magnitude of the coupling between the covalent and ionic surfaces. For example, at a total energy of 0.85 eV above the Na + I threshold, the period is 1.25 picosecond, the lifetime of the complex is 34 femtosecond, the recoil velocity is 0.0029 nm fs^{-1} and the reaction probability is 18%. That is, about one-fifth of the vibrations of the activated complex lead to reactants.

From such observations, one may determine that the covalent and ionic potential curves cross at an internuclear separation of 69.3 nm which is considerably different from the separation at the potential minimum of about 27 nm. The reaction intermediate is seen to vibrate, and as the internuclear separation approached 69.3 nm the complex may dissociate. However, not all complexes automatically dissociate. The results show that the molecule may reach the point of dissociation several times before breaking up. The period of this oscillation is 1.25 ps, Fig. 1 clearly shows that products are formed every 1.25 ps as molecules dissociate each time the internuclear bond is extended.

The gas phase photodissociation mechanisms of OClO in the near-ultraviolet have stimulated much in-

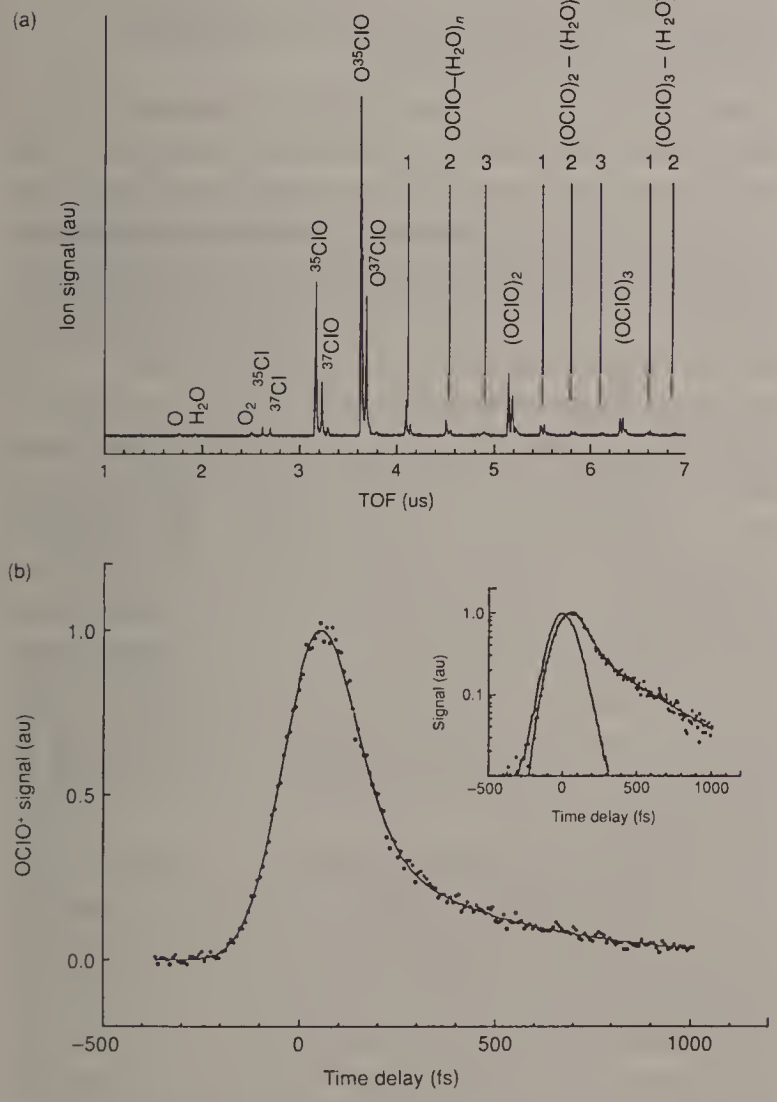


Fig. 2 Femtosecond dynamics (b) of the elementary fragmentation of OClO to OCl + O and to O + Cl + O. The time-of-flight mass spectrum (a) was recorded when the pump-probe delay time was near zero. Note that because of the femtosecond timing, the parent mass is the strongest peak. The observed decay is non-exponential (insert) and reflects the crossing of the wave packet to nearby potentials.

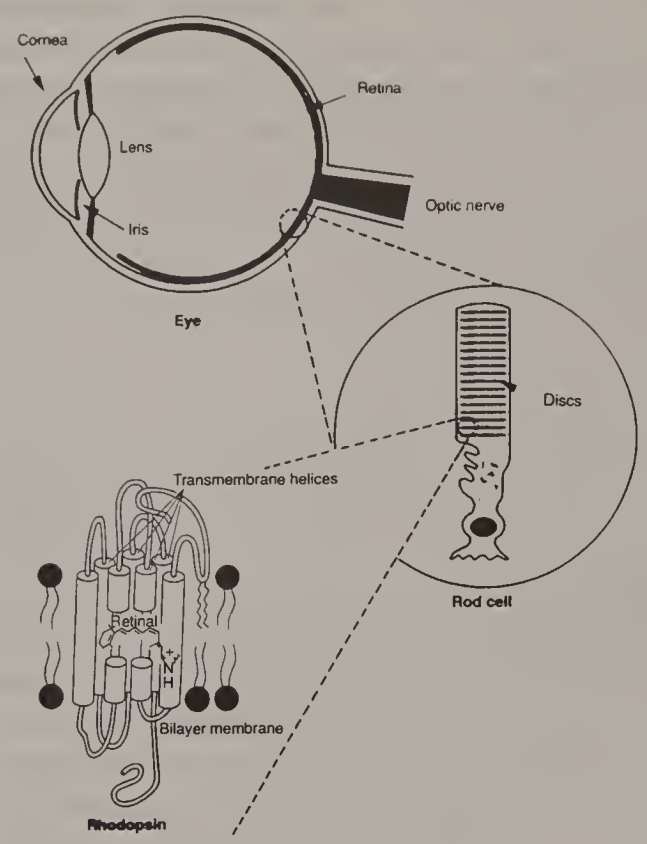


Fig. 3 The vertebrate eye produces images on the photosensitive layer of cells called the retina. The light-detecting protein, rhodopsin ($\lambda_{max} \approx 500$ nm), is located within the stack of disc membranes in the outer section of the retinal rod cells. The absorbed light isomerizes the bound 11-*cis* retinal chromophore to all-trans and thus initiates visual transduction.

terest as it is a reaction involved in the depletion of the ozone layer in the Antarctic stratosphere. At all wavelengths (475–273 nm), the major channel is found to be

$$OClO^* \rightarrow ClO + O,$$

whereas a minor channel is

$$OClO^* \rightarrow Cl + O_2.$$

The femtosecond dynamics of OClO elementary fragmentation were examined using FTS, see Fig. 2. Of particular relevance was the use of multiphoton ionization and mass spectrometry which made possible the observation of the parent ion of OClO. The nuclear motion was followed in real time and the dissociation pathways were monitored. For different levels of excitation of the symmetric stretching mode of the OClO molecule biexponential decays were observed of the OClO parent mass signal, see Fig. 2. The bond-breaking times are typically 300–500 fs (long decay component), while the faster decay ranges from 30–120 fs. The form of the transients and their change with energy reflects the nature of the reaction intermediates. The analysis of Zewail *et al.* considered the nearby potentials ($^2B_2$ and $^2A_1$) and the ground state ($^2B_1$) as the source of the vibronic interactions. In addition to the direct fragmentation to ClO + O, the dissociation proceeds through the intermediate $[OClO]^*_{e,\upsilon}$ (an electronically and vibrationally excited intermediate) to give the primary products ClO + O on the ground state and/or the minor products Cl + O_2 on the $^2B_2$ state. The elementary steps can be represented as follows:

$$OClO^* \rightarrow ClO + O$$

$$\rightarrow [OClO]^*_{e,\upsilon} \rightarrow ClO + O$$

$$\rightarrow Cl + O_2$$

The authors were thus able to map out the dissociation pathways of this triatomic molecule by directly probing the spectroscopy of the intermediate.

This chapter focuses attention on the concepts, techniques and several applications of femtochemistry. The chapter reviews studies of elementary and complex systems with special emphasis on fundamental concepts of reaction dynamics: (i) vibrational and rotational energy redistribution; (ii) state-resolved reaction rates; and (iii) the structure of the transition state.

The Chemistry Of Vision (Chapter 8, Prof. R.A. Mathies, Chemistry Department, University of California, Berkeley, USA).

It would be rather trite to say that the process of vision is one of our most common experiences, however, for all its importance and consequences it is a process which is not as yet fully understood. Mathies and his colleagues have used femtosecond spectroscopy to probe the primary event of vision, that is, the photoisomerization of the molecule rhodopsin. Fig. 3 shows where the light sensitive protein is to be found in the vertebrate eye. This protein has its absorption maximum at about 500 nm, which corresponds to about 2.5 eV or 20 000 cm^{-1}. This energy is absorbed by rhodopsin's 11-*cis* retinal prosthetic group (see Fig. 4) and initiates a photochemical *cis-trans* isomerization that results in the excitation of the retinal rod cell and visual sensation. The initial red-absorbing (about 550 nm) photochemical product, called bathorhodopsin, is thought to contain a distorted all-*trans* retinal chromophore.

The authors probed the photoisomerization process with femtosecond pulses as short as 10 fs (six fringes at 500 nm) and were able to observe that the isomerization was complete in 200 fs making it one of the fastest photochemical reactions studied. Such a rapid isomerization also implies that there is significant coupling between the excited S_1 state of the rhodopsin and the all-*trans* S_0 ground state, what the authors call a vibrationally coherent tunnelling process—see Fig. 4. After excitation, the photoproduct is formed in an essentially barrierless transition following the non-adiabatic potential surface indicated by the dashed lines in Fig. 4. The non-adiabatic surfaces carry the wave

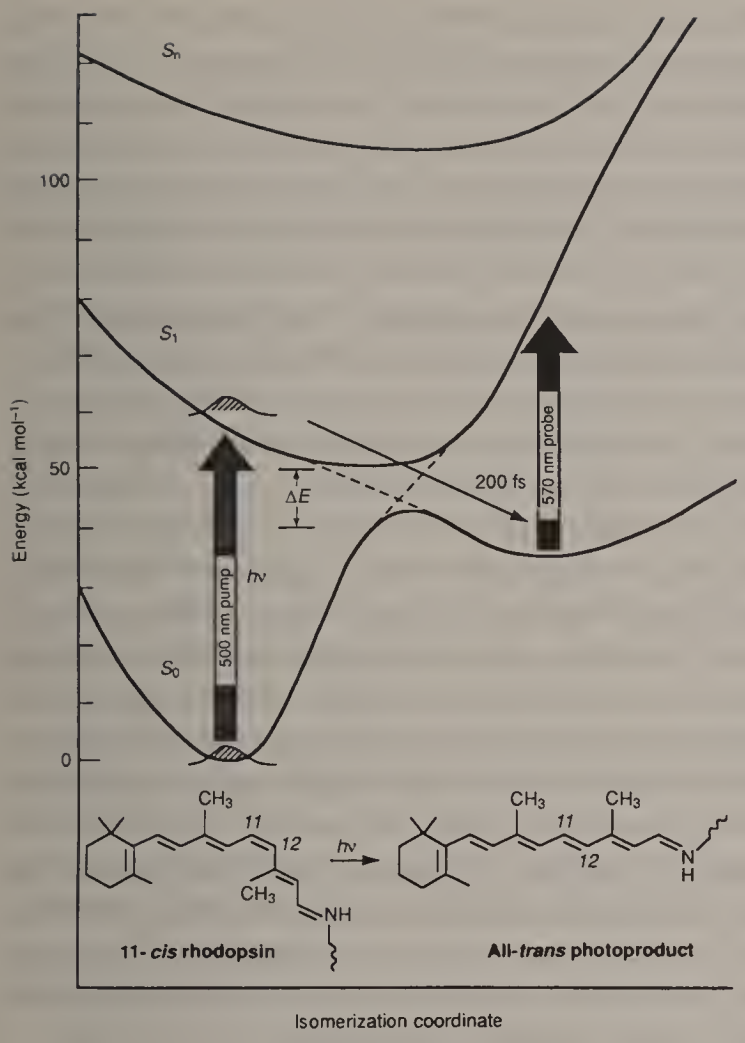


Fig. 4 Schematic ground- and excited state torsional potential energy surfaces for the 11-*cis* to all-*trans* isomerization in rhodopsin. The reaction path of the photoisomerization is indicated by the non-adiabatic potential surface (—).

packet rapidly and directly from the excited state of the reactant to the ground state of the photoproduct.

Mathies and colleagues have considered the theoretical implications of this work and have produced a new paradigm for visual photochemistry which may have relevance for a wide range of efficient photobiological processes.

With such femtosecond resolution, one has achieved almost the limiting time scale available for the study of reaction kinetics. As Nobel laureate Sir George Porter has said 'The study of chemical events that occur in the femtosecond time scale is the ultimate achievement in half a century of development and, although many future events will be run over the same course, chemists are near the end of the race against time.'

Not only are femtosecond pulses able to probe structures which exist only for the briefest of moments. Even if the femtosecond pulse is not resonant with the species of interest, one may still use nonresonant interactions to probe molecular dynamics on very short time scales. For example, the dynamics of solvent motion occur on a continuum of time scales, with the advent of ultrafast lasers, new approaches for probing motions on a time scale up to femtoseconds have become possible. In the optical Kerr effect, the molecules under study does not absorb a femtosecond photon, but oriented through the torque exerted by the electric field of the photon on the anisotropic polarizability present in the target molecule—a molecule such as CS_2 has a polarizability parallel to its main rotational axis ($\alpha_{\parallel} = \alpha_{zz}$) very different from that perpendicular to its main rotational axis ($\alpha_{\perp} = \alpha_{xx} = \alpha_{yy}$). This difference in components of the molecular polarizability is defined as the anisotriopy of the polarizability of the molecule, $\Delta\alpha = (\alpha_{\parallel} - \alpha_{\perp})$.

Optical Kerr effect studies of molecular dynamics

Of considerable current interest is the use of the optical Kerr effect to investigate liquid and solution structure and the localised motions of molecules in condensed phases. When a very short pulse of intense light passes through a fluid composed of anisotropically polarizable molecules it produces a transient birefringence—the optical Kerr effect. The development of powerful femtosecond laser pulses has lead to a new field of experimental investigation of molecular dynamics in both pure liquids and in solutions. For example, it is seen that the reorientational dynamics for an anisotropically

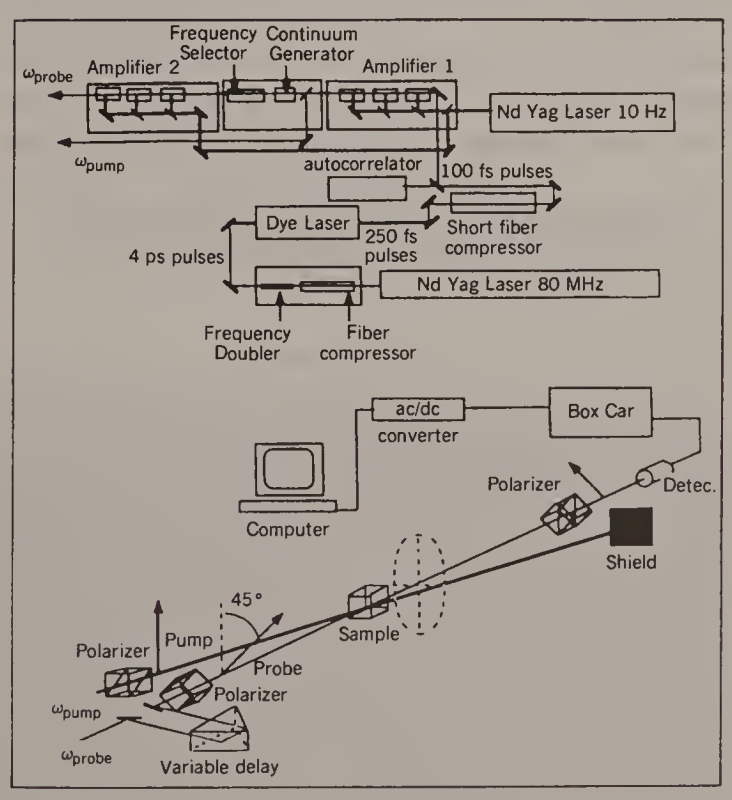


Fig. 5 Schematic drawing of a typical femtosecond optical Kerr effect laser system (the TROKE experimental setup at the European Laboratory for Nonlinear Spectroscopy, Florence Italy), the upper part of the figure give the details of the laser pulse generating and amplifying system and the lower part of the figure shows the relative polarizations of the pump and probe laser beams. Reproduced by kind permission of the *Journal of Chemical Physics*.

polarizable target molecule, in a strongly associated electrolyte solution, exhibit time scales for relaxation extending into hundreds of picoseconds. Whereas carbon disulphide molecules in pure CS_2, or in solutions of CS_2 in alkanes, are seen to reorient in 1.6 picoseconds.

In Fig. 5 we display an apparatus used for making measurements of the optical Kerr effect with pulsed lasers. A powerful laser pulse is generated which on passage through a polarizable medium induced a transient birefringence. The passage of this orienting pump pulse is quickly followed by a weaker probe laser pulse which samples the induced anisotropy. In Fig. 5, the pump and probe lasers are generated from the same source to reduce any temporal jitter (which is of some importance when dealing with such short pulses) between coupled laser sources and have the same wavelength. With the impressive temporal resolution of such equipment it has been observed, for example, that the transient induced optical Kerr effect in liquids of small polyatomics, e.g. CH_2Br_2 and CS_2 is structured. To interpret these latter measurements, a model has been proposed in which the reorientational dynamics of a molecule in such a weakly associated, covalent, fluid, as probed by the transient optical Kerr effect, consists of five dynamically distinguishable contributions. These are: (a) a purely electronic hyperpolarizability, that is, the electronic response of the molecules to the intense electric field of the laser (in such experiments the applied laser field is of order 10^7 Vm^{-1}). Secondly, (b) a rapidly dephased, coherently excited by the laser, intermolecular librational motion, the rocking of one molecule within the cage of molecules which surround it with a reorientational time of < 170 fs and occurring in a frequency regime 25–60 cm^{-1}. Component (c) is an intra-molecular vibrational contributions, corresponding to vibrational frequencies in the hundreds to few thousand wavenumbers. At longer times, (d) local translational fluctuations of the center-of-mass decaying over, typically 400 fs, which correlates with density fluctuations and hence to the time dependence of the solvent cage; consequently, correlated to the collision-induced anisotropy in the molecular polarizability. Finally, (e) a long-time reorientational anisotropy with a time scale for decay of about 1 ps.

The solvation dynamics of CS_2 in alkanes is consistent with the picture of a liquid as an ensemble of continually evolving, van der Waals-like solvation clusters; for which femtosecond and picosecond probing times reveal several discrete molecular motions. Molecules are seen to become trapped in locally ordered intermolecular potentials where they display motions which are characterised by specific frequencies and relaxations times. By contrast, in strongly associated liquids, for example, aqueous and methanolic solutions, it is seen that rotational reorientation dominates the observed optical Kerr effect measurements with timescales running into hundreds of picoseconds.

Ultrafast Processes in Chemistry and Photobiology, eds M. A. El-Sayed, I. Tanaka, Y. Molin. Blackwell Science, 1995, xiv + 306 pp., ISBN 0-86542-893-X, USD75. This book is published as part of the Chemistry for the 21st Century series of monographs by IUPAC.

New publications

IUPACSEARCH Version 4.1

Free computer disks containing all IUPAC recommended nomenclature and symbols and technical reports published in *Pure and Applied Chemistry* from 1960 through the end of 1994 are now obtainable from the IUPAC Secretariat. The disks are 3½ in., high-density, IBM-PC compatible format and will run under DOS (version 3.3 or later) or Windows. A hard disk with 5 Mb of free space and 640kb or greater of RAM are required. The software is easy to use and allows for Boolean searches; it is menu-driven and easy to use. Both colour and mono monitors are supported. Sorry, a Macintosh version is not available.

Please Fax or E-mail your request to: Mrs Gywneth Pettit, Fax: +44 (0)1943 880310;
E-mail: acadsoft@bsc.org.uk

Methods to Assess the Effects of Chemicals on Ecosystems

This volume in the SCOPE (Scientific Committee on Problems of the Environment) series of volumes presents methods to study the effects of chemical and physical agents on ecosystems in order to collect information that facilitates risk-based decisions.

Numerous chemical and physical agents, both man-made and naturally occurring in the environment, are capable of causing damage to ecosystems by, for example, altering their structure and function. The com-

plexity of the field and its rapid development, make it difficult to integrate this information into ecological management systems.

SCOPE 53 covers a discussion of the conceptual approaches to conducting ecological research and monitoring that includes: 'healthy' systems, setting and maintaining objectives for ecosystem management, and using ecological risk assessment as a model for studying the effects of chemicals on ecosystems. This volume provides an overview of available methods of studying the effects of chemicals on a variety of different ecosystems, for example, freshwater, brackish, estuary and near-coastal, forest and semi-arid. Ecological impacts on a regional scale are considered as well as the estimation of damage to ecosystems and approaches to integrating socio-economic concerns in ecological risk assessment.

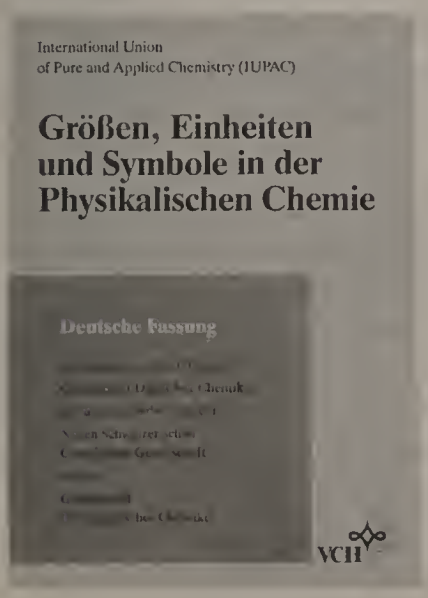
Ecological risk assessment is a useful framework to make decisions and to design monitoring programs that contribute to environmental policy and management decisions. Identifying ecosystem values, reference conditions and scales of interest are important first steps in the environmental risk assessment process that will guide the selection of monitoring methods.

This volume, a joint report summarizing findings and recommendations, followed by 14 contributed papers from experts of international repute, should be of interest to environmental regulators and to industries well as to researchers in the field of ecotoxicology.

SCOPE 53—Methods to Assess the Effects of Chemicals on Ecosystems, edited by R.A. Linthurst, P. Bourdeau and R.G. Tardiff is published by John Wiley & Sons Ltd, Baffins Lane, Chichester PO19 1UD, UK. ISBN 0 471–95911–1, price GPB 50.

Grössen, Einheiten und Symbole in der Physikalischen Chemie—the Green Book in German.

The Green Book is a compilation of **Quantities, Units and Symbols in Physical Chemistry**, edited by I. Mills, T. Cvitaš, K. Homann, N. Kallay and K. Kuchitsu, is currently in its second edition (ISBN 0632035838) and available from Blackwell Science at USD21 (full price) or USD 12.60 with an IUPAC discount. It has proven to be a most helpful collection of advice that is probably to be found on the desk of most physical chemists.



Recently, a German translation (ISBN 3 527 29326 4) of the second edition of this compendium has become available. This translation is available from VCH Verlagsgesellschaft mbH, Boschstrasse 12, D-69469 Weinheim, Germany, priced 58 DEM.

Grössen, Einheiten und Symbole in der Physikalischen Chemie, übersetzt von M. Hausmann, herausgegeben von K.-H. Homann, im Auftrag der Gesellschaft Deutscher Chemiker in Zusammenarbeit mit der Neuen Schweizerischen Chemischen Gesellschaft und der Gesellschaft Österreichischer Chemiker.

Unentbehrlich für jeden Chemiker—die offiziellen IUPAC-Richtlinien in deutscher Sprache.

Viele Fehler und Missverständnisse könnten vermieden werden, wenn man sich an eine einheitliche Terminologie und Symbolik hielte – und wünscht sich nicht jeder, Lernender wie Lehrender, ein wenig Hilfestellung in Zweifelsfällen? Dieses Buch enthält als 'letzte Instanz' die offiziellen IUPAC-Richtlinien: Kompetent, zuverlässig und vollständig gibt es Antwort auf fast alle Fragen zu Begriffen, Definitionen und Schreibweisen in der Physikalischen Chemie. Jeder, der ein naturwissenschaftliches Manuskript verfassen oder verstehen möchte, wird dieses Buch gerne zu Rate ziehen.

International Association for Cereal Science and Technology (ICC)

At the ICC General Assembly, held during the ICC Jubilee Confernce 1995, six new ICC Standard Methods were adopted. This now brings to 54, the number of ICC Methods available, there are also four ICC Recommendations. ICC Standard methods are available in English and, partly, in French and German. The complete 1995 Edition is priced at USD300.

Information about ICC and ICC Standard Methods may be obtained from:

International Association for Cereal Science and Technology Secretariat,
PO Box 77, Wienerstrasse 22A,
A-2320 Schwechat, Austria
Tel.: +43 1 707 7204; Fax: +43 1 707 7202

International Union of Biochemistry and Molecular Biology (IUBMB)

Compendium of Biochemical Nomenclature 1992

This volume has been prepared for IUBMB by Claude Liébecq, past chairman of the its Committee of Editors of Biochemical Journals. The compendium contains most of the nomenclature documents published in the first edition (1978), updated if subsequently revised; it also contains the new documents published since 1978 and references to other important nomenclature documents.

Biochemical nomenclature and related documents. A compendium, 2nd Edition (C. Liébecq, ed.), Portland Press Ltd, London 1992, ix+347 pages, ISBN 1 85578 055 4 (price USD36).

Enzyme nomenclature 1992

Since the publication in 1984 of the *Recommendations of the Nomenclature Committee of the International Union of Biochemistry* on the nomenclature and classification of enzyme-catalysed reactions, three supplements of corrections and additions to the enzyme list have been published in the *European Journal of Biochemistry*. These changes have been incoroprated, together with further amendments and additions, into the 1992 edition.

The new enzyme list contains 3384 entries, of which 314 are cross-referenced to deleted or transferred entries, leaving 3070 live entries—a 24% increase on the previous edition. Additions and changes are spread throughout the various types of enzymes, however, one group has undergone a particularly thorough revision—section EC3.4, the peptidases.

Enzyme nomenclature. Recommendations (1992) of the Nomenclature Committee of the International Union of Biochemistry and Molecular Biology, Academic Press Inc., San Diego, CA, USA 1992, xiii+862 pages. ISBN 0 12 227165 3 (paperback), price USD55.

Proceedings of the workshop 'Quantitative Structure Activity Relationships for Biodegradation'

W.J.G.M. Peijnenburg[1] and W. Karcher[2]

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Large numbers of hazardous organic compounds are emitted into the environment from anthropogenic and natural sources. Assessment of the ecological impact of the production and use of chemicals, necessitates available simple models that can be used to both qualitatively and quantitatively describe their fate and behaviour in the environment. Up till now, several of the transport and transformation processes that may contribute significantly to the removal of xenobiotic compounds from distinct environmental compartments have been studied in detail and various models and process descriptions are available. Several reaction paths have been investigated intensively and an increasing number of reaction rate constants can now be estimated quite accurately using a variety of Quantitative Structure Activity Relationships (QSARs).

For most organic chemicals, biodegradation is the dominant transformation pathway, contributing significantly to the attenuation of their environmental concentrations. However, due to the complexity of the biodegradative pathways, it only to a limited extent possible to extrapolate results of biodegradation tests obtained in the laboratory to realistic environmental field conditions; methods for predicting rates of biodegradation seem to be lacking completely.

In this present workshop it was proposed to bring together several international experts of several disciplines (for instance microbiology; environmental, physical and theoretical chemistry, and ecotoxicology) to discuss the present state of knowledge regarding biodegradative transformation pathways and the methods available to predict rates of biotransformation of organic compounds, and to give recommendations on the use of QSARs for predicting the course of biodegradative transformation pathways under realistic environmental circumstances.

Items to be addressed.

1 Introduction—general review of QSBRs.
2 Which test methods are available (for instance OECD-tests) and what type ofbiodegradation data are available for deriving QSBRs, and how can data published in literature be made available for deriving QSBRs.
3 A review of appropriate descriptors such as topological indices and quantum chemically derived descriptors.
4 'Techniques'; linear regression, Principle Components Analysis, Factor Analysis, Neural Networks, etc.
5 Results of QSBRs derived: (i) Using experimental data (ii) using expert judgement.
6 Mechanistic approach: (i) Review of degradation routes (ii) Development of QSBR models based upon the mechanism of degradation of similar compounds, for instance halogenated aliphatic hydrocarbons.
7 'Degner' approach; results for various subclasses of chemicals, not being based on the underlying mechanism but based on results from literature.
8 How to extrapolate the results obtained to field conditions.

The main finding of the workshop was that at first glance, biodegradation seems to lack order. Nevertheless, several models for predicting the course of biodegradative pathways have been reported. A limited number of these models are suited for use in risk as-

sessment or priority setting.

It was concluded that there is a lack of reliable and consistent data that can be used to derive new predictive models for biodegradation. There still is insufficient knowledge of the basic processes that take place during biodegradation, and the influence of environmental conditions. This severely hinders the extrapolation of results obtained in the laboratory to realistic field conditions. In the near future, the major advancements should be expected in the standardisation and unification of biodegradation tests as well as biodegradation data. This will strongly facilitate the development of new models for environmentally relevant biodegradation end-points.

It is recommended that in future work more attention should be devoted to better understanding of the process modelled. One of the procedures would be to start at the basic level of biodegradation: modelling the biotransformation reactions at the enzymatic level, and subsequently follow a stepwise approach towards understanding of the same reactions at the microbial level in the 'real' environment.

Recommendations:

1 With the aim of increasing the knowledge of the underlying processes, the approach suggested by Damborsky was supported: Derive QSARs for enzymatic processes, on the basis of modelling of chemical conversions inside the active site of enzymes. The underlying hypothesis is that there are less enzymes than organisms, and one should be aware that biodegradation is not a discontinuous process. Subsequently, a step-wise approach towards understanding the interactions at the microbial level in the 'real' environmental should be followed. As an additional recommendation it was suggested to include information on metabolic pathways, as presented by Muller.

2 The future developments in qualitative and quantitative structure-biodegradability relationships primarily depend on availability of high quality experimental biodegradation data, obtained either by the evaluation of existing data or by measuring new data. Thus, in the near future, the major advancements should be expected in the standardization and unification of biodegradation tests as well as biodegradation data.

3 The environmental conditions can be as important as structure in determining the outcome of a biodegradation test. At present, a single laboratory test (OECD closed bottle test in Europe and 20 days BOD test in US) is used to evaluate ultimate biodegradation of commercial chemicals in all environmental conditions. It is difficult to imagine that a single test can and should reflect all possible real environmental conditions. It is reasonably to assume that under different environmental conditions different processes (reactions) will be the rate determining step for biodegradation, i.e. hydrolysis, oxidation, dehalogenation, or similar. It is also possible that the nature and activity of the microorganisms involved in degradation may be a rate determining step. Thus, different environmental scenarios should be described and defined by the minimal set of necessary physical and chemical conditions. Ideally, the influence of critical biological or biochemical parameters like co-factors, co-metabolism, and others should also be assessed. From each set of 'standard' conditions, it must be possible to determine which process (reaction) will be a rate determining step. Also, the hierarchy of degradation processes (reactions) must be constructed for each environmental scenario. Thus, the present question on environmental degradation 'will a chemical biodegrade rapidly or slowly?' should be formulated as 'will a chemical biodegrade rapidly or slowly under the following set of (field) conditions: (a) physical (b) chemical (c) biological, etc.?'

This report is prepared within the framework of the project 'Quantitative Structure–Activity Relationships for Predicting Fate and Effects of Chemicals in the Environment', supported by the Environmental Technologies RTD Programme of the Commission of the European Communities. The workshop on 'Quantitative structure activity relationships for biodegradation' was also supported by IUPAC/ICSU and was held in Belgirate, Italy, in September 1994. Copies may be purchased from Mr J. Winters, National Institute for Public Health and Environmental Protection, PO Box 1, 3720 BA Bilthoven, The Netherlands (Fax: +31 30 274 4404). The price is NLG47.20. If ordering, please quote Report Number 719101021.

The Silver Book—the latest in the Nomenclature Series

Compendium of Terminology and Nomenclature of Properties in Clinical Laboratory Sciences (Recommendations 1995)

Over the last 40 years, much effort has been made to introduce and apply in clinical chemistry the rules and conventions on quantities and units recommended by international organizations such as BIPM, ISO and IUPAC.

The series of documents and recommendations published for this purpose by IUPAC/C-QUCC and IFCC/C-QU (formerly IFCC/EPQU) are not readily available, and some have been in need of updating and alignment with other

documents. This Compendium, the Silver Book, harmonizes them, and will facilitate access and updating.

History of recommendations on quantities and units in clinical chemistry

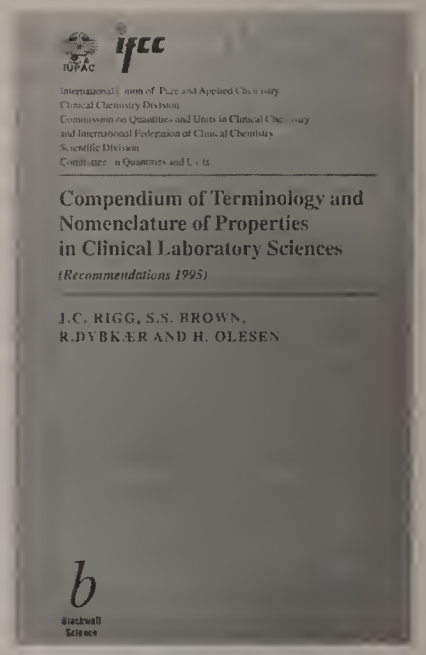
The beginnings of the work on quantities and units in clinical chemistry illustrate the catalytic interplay of international organizations, national societies and individuals with new ideas.

In 1954, the 10th General Conference on Weights & Measures (CGPM) met and resolved that 'In accordance with the wish expressed by the 9th CGPM, of 1948, in its Resolution 6 concerning the establishment of a practical system of units of measure for international use, the 10th CGPM decides to adopt as base units: metre, kilogram, second, ampere, degree Kelvin, and candela. In 1960, that system became known as the International System of Units. In 1971, the mole was added to the system on the advice of the International Union of Pure & Applied Chemistry (IUPAC), the International Union of Pure & Applied Physics (IUPAP) and the International Organization for Standardization (ISO).

In the late 1950s, probably most chemists and certainly most scientists in biologically oriented disciplines dismissed the recommendations on weights and measures as irrelevant, of concern only to physicists and engineers. As parts of ISO Recommendation 31 (the forerunner of ISO31 1992) on quantities and units were being published up to 1960 on 'periodic and related phenomena', 'mechanics' and 'heat', their opinion of its irrelevance would probably have been confirmed. The titles suggested that such recommendations were not interdisciplinary.

In 1952, an IUPAC Commission on Clinical Chemistry had been formed to coordinate national groups. A professor from Geneva, Manuel C. Sanz, predecessor at the University of Geneva of another worker for the International Federation of Clinical Chemistry (IFCC), Marc Roth, encountered a group of young medical graduates during a visit to Copenhagen. The group was pursuing further studies in biochemistry, including analytical, inorganic, organic and physical chemistry. Sanz became aware of the local ideas on working towards a unified 'presentation of results' in clinical chemistry and took immediate steps to bring their ideas to the attention of the international scientific community.

In 1957, René Dybkaer had been invited by the Danish Society for Clinical Chemistry & Clinical Physiology to give a paper entitled 'Standardizing unit symbols in work of the clinico-chemical laboratory'. It was a plea for implementation in clinical chemistry of the recommendations of the IUPAC 'Commission on Symbols and Physicochemical Terminology' and of ISO Technical Committee 12 on quantities and units.



The strength of the beginnings in Denmark was the realization that the recommendations of the International Bureau of Weights & Measures (BIPM) and ISO, despite their orientation to physical sciences, had an interdisciplinary element that needed to be sought out and applied. The Danish Society appointed a committee which presented a proposal in 1960 to the other Scandinavian societies of clinical chemistry, and also translated it as a proposal to the Fourth International Congress on Clinical Chemistry in Edinburgh in 1960. The IUPAC Commission on Clinical Chemistry referred the proposal to the Fifth International Congress in Detroit in August 1963. Meanwhile, ideas were developing further in Scandinavia. The relevance of molecular quantities, though not then part of the International System, was stressed.

The Committee on Standards & Control of the American Association of Clinical Chemistry discussed the proposal in 1963 and its comments formed part of the subsequent recommendation. The situation as seen from the United States is described by Radin (1967). 'A system of units for clinical chemists was proposed by the Danish Society for Clinical Chemistry and Clinical Physiology. This system was transmitted to the IUPAC Commission on Clinical Chemistry in June 1963. A Subcommittee on Nomenclature & Usage of the Committee on Standards & Controls of the American Association of Clinical Chemistry was assigned the task of studying the problem with a view to agreement upon a set of rational and internally consistent objectives for nomenclature reform. The recommendations of the subcommittee were in close agreement with those of the original Danish proposals as being desirable objectives.'

The proposal was accepted as a basis for a recommendation at the Fifth International Congress, where a symposium was held on 'Nomenclature and standard units'. The draft recommendation was presented to the IUPAC Commission on Clinical Chemistry in 1964.

At the IUPAC General Assembly in Paris in 1965, the Commission resolved to recommend the litre, rather than the SI unit, the cubic metre, as the denominator unit in expression of concentrations, and appointed a Subcommission for Standards and Units in Clinical Chemistry.

The principle of preference for amount-of-substance approved in 1966 was ratified in 1972 by the International Committee (now Council) for Standardization in Haematology (ICSH), IFCC and the World Association of Societies of Anatomic & Clinical Pathology (WASP). The recommendation was published in 1973, together with one on preference for the litre in expression of concentrations, under the title 'Use of SI in clinical laboratory measurements'. By 1967, the concepts of amount-of-substance and its unit the mole were close to recognition by the international metrological authorities. The recommendations of IUPAC and IFCC on those subjects are still largely valid.

Two sections of the 1966 draft failed to reach approval: 'Whole number measurement of quantities' and 'Qualitative measurement of quantities'. These issues have continued to plague the reporting of analytical data and have surfaced again in discussions in recent years.

In 1971, the IUPAC Commission and IFCC Expert Panel (which became a Committee in the 1980s) published two of the most useful guides on the reporting of biological and chemical data, the IUPAC 'Yellow Appendices' nos 20 and 21 of 1972 (IUPAC Information Bulletin. Appendixes on Nomenclature & Terminology), which were a provisional abridged revision of the 1966 recommendations. Revision of them began during the IUPAC General Assembly at Munich in 1973.

The group met at Munich again in 1974. Besides the revision of the 1967 publication, of which the Yellow Appendices 20 and 21 were the first stage, drafts were discussed on fluid mechanics, on spectroscopy and on chemical activities and pH. The discussions were extremely thorough.

By contrast with that rapid progress towards agreement among clinical laboratory scientists on ways of expression of concentrations, the problems of expression of enzymological data were just being realized for the first time. Dybkaer had a seemingly endless itinerary in the early 1970s discussing enzyme activity and catalytic amount, and their units the enzyme unit and the katal, with ISO Technical Committee 12, the IUPAC/International Union of Biochemistry (IUB) Joint Committee on Biochemical Nomenclature and the authorities of IUPAC and IFCC. The problems were resolved by CQUCC and EPQU and the IFCC Expert Panel on Enzymes at a joint meeting at Strasbourg in 1975. The results of the negotiations with the Joint Committee on Biochemical Nomenclature of IUPAC and IUB were published in 1978. A revised version of the recommendation of the commission and expert panel was published in 1979. However, despite a petition from IUPAC and IFCC to the International Bureau of Weights & Measures, the katal was never recognized as a base unit of catalytic amount, though in the same period radiologists managed to win approval of special names for the derived units becquerel, gray and sievert with similar arguments about human safety.

At the IUPAC General Assembly in Madrid in September 1975, there were joint meetings with the two spectroscopic commissions of IUPAC, who tore to pieces an early draft on quantities and units in spectroscopy: but logical, user-friendly answers were still-needed. The discussion with the physical chemists yielded permission to introduce the term **substance concentration** instead of the long-winded **amount-of-substance concentration.** However, discussion on whether the unit of catalytic amount, called the katal, was a base unit or a derived unit was extremely heated. The members of the Commission were sent away with instructions to introduce the new nomenclature properly. At times, that project was extremely frustrating, despite the encouragement of a subsequent chairman of IDCNS, Norman Jones, who prophesied rightly that it would take at least another 10 years. Surprisingly, one of the more trivial words of those first suggestions, **attenuance,** has become popular. The group's understanding of dimensional analysis was questioned at Madrid, but it has proved a useful tool to bring together many quantities currently known under a variety of names.

In the 1970s, metrologists and the physical chemists at Madrid looked askance at the distinction Dybkaer and Jorgensen had made in 1967 between quantity (now called **measurable quantity** by the International Vocabulary of Metrology, VIM) and **kind-of-quantity** (called *quantity in a general sense* by VIM). By contrast, three past members of IUPAC-CQUCC and IFCC-EPQU have recently participated in the committee of an ISO task group responsible for revising VIM (BIPM *et al.* 1993). Clinical laboratory sciences are now being taken seriously as a branch of metrology.

The need for clarity of intergovernmental policy on SI in the medicinal professions led to the preparation by the World Health Organization (WHO) of a guide to international recommendations on names and symbols for quantities, and on units of measurement (WHO 1975), in which the group provided considerable information about IUPAC and IFCC recommendations. This led to a resolution of the 30th World Health Assembly (WHA) at Geneva in May 1977. The group, in particular its chairman, Robert Zender (la Chaux-de-Fonds, Switzerland), advised on the formulation of the recommendation and on the subsequent publication by WHO (1977) of a booklet on SI in the medical professions, as requested by the 30th WHA. There had been strong requests, notably from cardiologists, for clarification of policy on units for blood pressure, and that issue was clarified for the time being in a resolution of the 34th WHA in 1981.

A recent issue worked out jointly between the group and WHO experts on biological standards has been the

metrological status of WHO International Units and the problems of using biological reference materials as standards in biological, immunological and chemical measurements.

Introduction of the general language of metrology into a biologically oriented discipline has been a two-way process. One example was the deficiencies found in the names of spectrometric quantities. The resulting thorough critique seriously delayed the publication of a recommendation on absorption spectrometry, which was finalized jointly with the IUPAC Commission on Molecular Structure & Spectroscopy. However, it did force the commission and expert panel to initiate a separate project on nomenclature of derived quantities (IUPAC-CQUCC and IFCC-CQU 1991), which was finalized by H. Peter Lehmann (New Orleans, Louisiana, United States), who took over as chairman in 1979. That recommendation considerably influenced the nomenclature of ISO-31 1992.

At the IUPAC General Assembly in Hamburg in 1991, it was suggested that the time was ripe to consolidate the recommendations from the Division of Clinical Chemistry. Several of the initial members of the group on quantities and units in clinical chemistry were still active and could still be consulted. Several of a new generation of recommendations were near to finalization. Two key members of the group from the early 1970s had died: Roland Herrmann, who initiated the work on spectrometric quantities, in 1980; and Pierre Métais, who did much to standardize nomenclature and use of quantities in the French-speaking world, in November 1987.

A history is not complete without a word about the correspondents from many parts of the world, some irate or emotional, others coldly logical. There were hundreds of comments from individual scientists and from manufacturers. Others represented organizations, including:

- other groups within IUPAC and IFCC, in particular the IUPAC InterDivisional Committee on Nomenclature & Symbols, Commission I.1 on Physicochemical Symbols, Terminology & Units and the two commissions on spectroscopy;
- national societies of clinical chemistry, in particular the American Association of Clinical Chemistry;
- other scientific unions or medical societies, in particular the International Union of Biochemistry and Molecular Biology (IUBMB, formerly called the International Union of Biochemistry, IUB), the International Council (formerly Committee) for Standardization in Haematology (ICSH) and the World Association of Societies of Anatomic and Clinical Pathology (WASP);
- intergovernmental organizations, including WHO, ISO, BIPM and the International Organization for Legal Metrology (OIML);
- regional organizations, for example the Community Bureau of Reference (BCR), now called the Standards Measurements and Testing Programme of the European Union.

They have all played a role in the evolution of these recommendations.

Compendium of Terminology and Nomenclature of Properties in Clinical Laboratory Sciences (eds J.C. Rigg, S.S. Brown, R. Dybkaer and H. Olesen) Blackwell Science (Osney Mead, Oxford OX2 0EL); xi + 290 pp. (ISBN 0865 42 6120); Price USD28.50 (paperback). With the IUPAC discount for Affiliates, the price is USD17.10.

Affiliate Affairs

Information for affiliates

IUPAC publications

Affiliates are entitled to a 25% reduction, and in some cases a 40% reduction on the cost of IUPAC publications except *Pure and Applied Chemistry*. A leaflet detailing IUPAC books currently available from Blackwell Science Ltd has recently been distributed by the publishers to all *CI* readers. Further copies may be obtained from the IUPAC Secretariat.

How to contact commissions

IUPAC affiliates may if they wish communicate directly on scientific matters with the officers of IUPAC commissions. A full list of names and addresses of all commission officers for 1996–97 was published in the November 1995 issue of *CI*.

Affiliate reduction of conference registration fees

It is a condition of IUPAC sponsorship of a conference that IUPAC affiliates are entitled to a 10% reduction or 'own members' rate on the registration fee for scientific participants. This concession is usually, but not always, announced in the conference circulars and indicated on the registration form.

To receive this reduction an affiliate must declare on the conference registration form that (s)he is an affiliate. Alternatively the affiliate should apply in writing to the conference organizer for this reduction stating that (s)he is an affiliate. Conference organizers may check with the IUPAC Secretariat that applicants for this reduction are currently registered as affiliates.

Address of IUPAC Secretariat

Please use the following address for all communications directed to the IUPAC Affiliate Affairs Secretary. If your are submitting a letter for publication in *Chemistry International* (*CI*), please indicate that the letter is 'Submitted for publication in *CI*.'

Affiliate Affairs Secretary
IUPAC Secretariat, Bank Court Chambers
2–3 Pound Way, Templars Square
Cowley, Oxford OX4 3YF, UK.

Tel: +44 (1865) 747744
Fax: +44 (1865) 747510
E-mail: iupac@vax.oxford.ac.uk

If an application for this reduction is refused, an affiliate should immediately notify the Affiliate Affairs Secretary and, if possible, forward copies of documentary evidence of this refusal.

Ties and scarves

Ties and scarves emblazoned with the IUPAC logo may be purchased from the IUPAC Secretariat by applying to the Affiliate Affairs Secretary. The colours for both are *either* maroon *or* dark blue. The ties cost USD 14.00/GBP 7.00 each and the scarves USD 12.00/GBP 6.00 (including postage and packing).

Please use the form (or a photocopy of it) published on page 24 of the January 1994 issue of *CI*. Alternatively please write to the Affiliate Affairs Secretary with your order stating the colour you require. A cheque made payable to IUPAC for the appropriate amount should be enclosed with your order.

Visas

It is a condition of sponsorship that organizers of meetings under the auspices of IUPAC, in considering the locations of such meetings, should take all possible steps to ensure the freedom of all bona fide chemists from throughout the world to attend irrespective of race, religion, or political philosophy.

IUPAC sponsorship implies that entry visas will be granted to all bona fide chemists provided application is made not less than three months in advance. If a visa is not granted one month before the meeting the IUPAC Secretariat should be notified without delay by the applicant.

IUPAC poster

Copies of an IUPAC poster are available **free of charge** to affiliates and members of IUPAC's commissions and committees. The poster is printed in maroon and black on a white background and is approximately 42 × 59 cm in size.

IUPAC welcomes any publicity you can give to its activities. If you would like to display one or more copies of the poster in your department or elsewhere please write to the Affiliate Affairs Secretary stating your name and address and how many copies of the poster you wish to receive.

IUPAC-sponsored conferences

An updated list of names and addresses of the organizers of all future IUPAC sponsored conferences is given in the 'Conference Calendar' published in each issue of *CI*.

A Letter from Cuba

Alberto J. Nuñez Sellés

Chemistry and IUPAC Affiliation Membership Programme: improving chemists communication

Since 1988, Dr Alberto J. Nuñez Sellés has been the National IUPAC Affiliation Secretary in Cuba. As Director of the Center of Pharmaceutical Chemistry, and through his more than 20 years of experience in chemistry (organic synthesis, chromatography, mass spectrometry and organic trace analysis), he has an authoritative opinion about goals of Chemistry in Cuba and the operation of its IUPAC Affiliation Programme.

Cuban IUPAC Affiliates have increasingly been participating in national activities since the IUPAC Affiliation Programme started in early 1988. Initial expectation was surpassed and the increase from 25 to 35 affiliates in the past 2 years, through funds made available by UNESCO, was the main achievement. These chemists are representative of the youngest generation of teachers, technicians and researchers in Cuba and are actively involved on several chemistry and chemistry-related areas such as organic synthesis, chromatographic development, analytical chemistry, quality control and assurance, biotechnological applications, pollution control, waste treatment, etc. They are not only located in the capital city but distributed among the main centres of chemistry development (Santiago de Cuba, Holguin, Camaguey, Santa Clara, Pinar del Rio).

Knowing what are the various chemistry components in Cuba, it will be easier to understand how the IUPAC Affiliation Programme works and its results:

Chemistry R&D has been of increasing prioritary during the last years in national projects which cover practically all areas of chemistry. More than 100 R&D institutions exist in the country with *c.* 3000 chemists who are continuously developing new techniques and concepts or improving already existing processes in laboratories and industries.

Chemical production, focused mainly on sugar and sugar cane derivatives, is widely distributed in the country with more than 10 000 chemists working on chemical engineering, process and quality control, purification processes, etc.

Chemistry teaching in high schools and polytechnic institutes has increased in terms of quantity and quality during the last three decades. Around 5000 students in three Polytechnic Institutes of Chemistry (Pharmaceutical, Food and Sugar Chemistry) and a similar number in University Faculties of Chemistry and Chemical Engineering carry out their studies for graduate degrees. Both Universities and R&D institutions support postgraduate and doctoral studies on chemistry. Around 300 Cuban chemists hold a PhD degree or equivalent (*Doctor en Ciencias Químiças*).

In this context, the Cuban Chemical Society and its IUPAC Affiliation Secretary have a wide and strong basis for selecting critical areas of development, focused on the exchange of ideas, experiences, projects and expertise knowledge. As example; four main events in Chemistry have been successfully held in Cuba during the last years:

1 *'First, Second and Third Workshops on Scale-up of Drug Technologies: Chemistry, Biotechnology and Natural Products'*, Havana, April 1991, 1993 and 1995, organized by the Center of Pharmaceutical Chemistry and sponsored by the Ministry of Public Health, PAHO/WHO and UNDP, with 200 participants on each edition.
2 '*XIV Conference of Chemistry*' Santiago de Cuba, May 1995, organized by the University of Oriente and the Autonomous University of Mexico, with 500 participants and lecturers from USA, Mexico and Cuba.
3 '*Biotechnology*' Havana, November 1991, 1993 and 1995, organized by the Center of Genetic Engineering and Biotechnology and sponsored by several organizations, with more than 1000 participants on each edition and a significative foreign participation.
4 'Cuban School of Theoretical Chemistry', March 1992 and 1994, organised by the University of Havana and sponsored by several organizations with *c.* 100 participants from Latin American countries.

Cuban Affiliates are demanding to be more actively engaged on IUPAC activities. The question 'How to do it?' has been discussed at some length, but still remains unanswered. The following are just ideas of how IUPAC bodies and commissions could increase Affiliates activities considering geographical origin and country development:

- Nomination of Affiliates as IUPAC Officials or Representatives in Bodies and Commissions.
- Funding small projects (USD 5000 max.) to support participation of relevant young IUPAC Affiliates at IUPAC-sponsored events.
- Coordination of R&D Projects proposed by Affiliates from developing countries and support for their presentation to financing bodies.
- Organization of regional meetings of IUPAC Affiliates, organized and financed by the host country and supported by IUPAC, to exchange ideas about development of specific topics in chemistry and create a communication route for joint research projects within the geographical region.

The decision from the recent IUPAC General Assembly to continue AMP activities certainly will help promote this discussion of ideas on how to improve and encourage such activities. Future AMP activities seem to be promising and the Cuban chemical community is ready for this step. It would be an excellent opportunity to all Affiliates to reinforce communication and co-operation.

Havana
September 1995

Conferences

6th European Conference on Electroanalysis (ESEAC '96), University of Durham, Durham, UK, 25–29 March 1996

Topics for discussion include:

- Chemical Sensors, Arrays, Chemometrics
- New Technologies and Materials
- Environmental, Industrial and Clinical Applications

For further details, please contact:
Prof. A. K. Covington,
Department of Chemistry,
University of Newcastle,
Newcastle upon Tyne,
NE1 7RU, UK.
Tel.: +44 191 222 6785; Fax: +44 191 222 6929;
E-mail: a.k.covington@newcastle.ac.uk

How to apply for IUPAC sponsorship

To apply for IUPAC sponsorship, conference organizers should write to the IUPAC Secretariat (see inside back cover for address) requesting an Advanced Information Questionnaire (AIQ). Completed AIQs should be returned to the Secretariat preferably 2 YEARS and at least 12 months before the conference. Late applications will not be considered. Further information on granting of IUPAC sponsorship was published in *Chem. Intl.* **14**, 203 (1992).

7th International Conference on Multiphoton Processes (ICOMP VII), Garmisch-Partenkirchen, Germany, 30 September 4 October 1996.

IUPAC SPONSORED

Topics to be considered include, but will not be limited to the following:

- Multiphoton and tunnel ionization of atoms and molecules;
- Intense laser fields on atoms and molecules;
- Above threshold ionization;
- Coherent control of atomic and molecular processes;
- Multiphoton processes in molecules and Coulomb explosion;
- High order generation and XUV radiation processes;
- Ultrashort laser pulse effects on atoms and molecules;
- Relativistic effects in strong radiation fields;
- Multiphoton processes in clusters and macromolecules, and on surfaces.

The conference will take place at the Congress Center in Garmisch-Partenkirchen, a well known Olympic town which lies at the foot of Germany's highest mountain, the Zugspitze.

The conference registration fee is 450 DEM, if paid before 1 August 1996. Thereafter, the registration fee will be 500 DEM. The reduced registration fee for students is 150 DEM.

Information and the second circular may be obtained from the conference secretary:

Renate Weise-McKinght
Max-Planck-Institut für Quantenoptik
Hans-Kopfermann-Str. 1
D-85748 Garching
Germany
Tel.: +49 89 32905 736; Fax: +49 89 32905 200
E-mail: rwm@mpq.mpg.de

International Symposium on Food Packaging—*Ensuring the Safety and Quality of Food*, Budapest, Hungary, 11–13 September 1996

IUPAC SPONSORED

The International Life Sciences Institute (ILSI) is a worldwide non-profit foundation. ILSI Europe was founded in 1986 and provides a useful forum through which members of industry, experts from academia, together with medical and public institutions may address issues related to health and nutrition.

The present symposium will concentrate on reviewing the science necessary for further improvements in the quality of food packaging and the understanding of chemical and physical processes observed in food packaging systems. Microbiological and sensory considerations in developing packaging will also be discussed. The multidisciplinary meeting will be of interest to food scientists, chemists, mathematicians, physicists and microbiologists from industry, academia and government—all who are concerned with food safety.

The program will cover a wide range of topics related to food packaging:

- Packaging—improved safety and quality of food;
- Innovations in food packaging—modified atmosphere, edible, biodegradable and recyclable;
- Physical transport processes in packaging;
  (i) gas diffusion
  (ii) organic vapour permeation
  (iii) component migration of foodstuffs
  (iv) interface phenomena
- Sensory impact of packaging materials—taint;
- Functional barriers—theoretical approaches and performance testing;
- Safety/quality considerations for recycling and reuse;
- Component migration to foodstuff with high temperature applications;
- Alternative test procedures and new analytical approaches;
- Active and smart packaging;

The programme will consist of a number of keynote lectures together with contributes oral presentations and a poster session. The conference language will be English.

It is anticipated that the registration fee will be approximately 350 ECUs including admission to the symposium, lunches, one gala dinner, coffee/tea and the book of abstracts. A limited number of places are available for students at a reduced rate.

For further information, please contact:
Dr Laura Contor—ILSI Europe,
Avenue E. Mounier, 83—Box 6,
B-1200 Brussels,
Belgium
Tel.: +32 2 771 00 14; Fax: +32 2 762 00 44

International Conference—*Chemical Physics at the Border of the XXI Century*, Moscow, Russia, 16–19 April 1996

IUPAC
SPONSORED

This conference is being organized as one of the events to celebrate the memory of Academician N. N. Semenov, a Nobel Prize winner, on the occasion of his 100th birthday. Semenov's name is associated with a number of scientific areas. For example, he developed a general theory of chain reactions and the theory of explosions—he carried out fundamental research in chemical kinetics.

This conference will serve to discuss other essential achievements of Semenov and how they helped shape modern chemical physics.

The registration fee for participants and accompanying persons from Russia and the CIS is 50 000 Roubles, from other countries the fee is USD100. The languages of the conference will be English and Russian. Hotel accommodation and meals are not covered by the registration fee.

For further information, please contact:
Prof. V. Rochev Semenov Conference,
Institute of Chemical Physics,
Russian Academy of Science,
117977 Moscow, GSP-1, V-334,
ul. Kosygina 4,
Moscow, Russia
Fax: +7 095 9382156; E-mail: nns@chph.rc.ac.ru

2nd International Symposium on Free Radical Polymerization: Kinetics and Mechanisms, Santa Margherita Ligure, Genova, Italy, 26–31 May 1996

IUPAC
SPONSORED

This IUPAC-sponsored symposium is jointly organized by the Institute of Industrial Chemistry, University of Genoa, and the Institute of Physical Chemistry of Synthetic and Natural Macromolecules of the National Research Council of Italy. The symposium will be held in a small coastal town, Santa Margherita Ligura, in the Hotel Regina Elena.

The symposium hopes to review the current knowledge of free radical polymerization and copolymerization. Topics to be covered include: Chain transfer, modelling, photoinitiation, emulsion polymerization, copolymerization, etc.

The scientific program will consist of invited lectures as well as poster sessions of accepted contributed papers. The symposium is organized as a discussion meeting, based on nine scientific sessions and centered on 27 invited lectures. There will also be a poster presentation covering specific aspects of both pure and applied research in the field of free radical polymerization. The symposium language will be English.

The registration fee is 770 000 ITL for active participants, 350 000 ITL for student participants and 300 000 ITL for accompanying persons. Accomodation is available at the Hotel Regina Elena.

For further information, please contact;
Prof. S. Russo
Instituto di Chimica Industriale
Università di Genova
16132 Genova,
Italy
Fax: +39 10 353 8323; E- mail: russo@cisi.unige.it

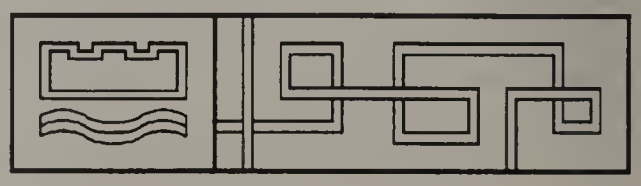
11th Bratislava Conference on Polymers: Thermal and Photo-induced Oxidation of Polymers and its Inhibition in the Upcoming 21st Century, High Tatras, Slovak Republic, 23–27 June 1996

IUPAC
SPONSORED

This microsymposium is intended to bring together scientists from academic and industrial institutions to discuss recent progress in the chemistry and physics of polymer oxidation and stabilization and to consider how the field may develop in the next century.

The following topics will be covered:

- The development of our understanding of photo and thermal oxidation of polymers, polymer composites and polymer blends, together with strategies for their stabilization.
- The effect of hydroperoxides, aldehydes, trapped free radicals and reactive components in either heterogeneous or homogeneous reaction systems on the kinetics of degradation and the efficiency of stabilizers.
- Development in methods for studying photooxidation and thermally induced oxidation



(surface analysis, FTIR and other spectroscopic probes, chemiluminescence techniques, chemical methods of analysis of oxidation products, etc.).
- Computer simulation and modelling of oxidation under heterogeneous and homogeneous conditions.

The program will consist of main lectures, contributed lectures and posters. The conference language will be English. The symposium is being held in the Hotel Academia which is located in the eastern part of the National Park of the High Tatras.

The registration fee (not including accommodation) is 380 CHF for active participants, 340 CHF for IUPAC Affiliates, 240 CHF for students and 150 CHF for accompanying persons.

For further information, please contact:

Dr Lyda Rychlá, Polymer Institute of the Slovak Academy of Sciences,
Dúbravská cesta 9,
842 36 Bratislava,
Slovak Republic
Tel.: 0042 7 37 34 48, Fax: SAVPOLYMER Bratislava 0042 7 37 59 23
E-mail: upolrych@savba.sk

6th International Energy Conference and Exhibition (Energex '96), Beijing, China, 3–7 June 1996

Energex '96, an international energy conference and exposition will be held in Beijing in June 1996, in cooperation with a host of sponsors from within China and from around the world.

The combined body of scientific knowledge and its transfer to industrial growthand prosperity is an integral part of technological advance by all nations. The Energex '96 confernce will provide a vehicle for the exchange of professional expertise and transfer of technology by one-to-one interaction between energy researchers and industrial representatives from all nations. The confernce will provide a window of opportunity for industry, research institutes and others to promote their capacity and cabaility, and also to establish key contacts with their counterparts from within China and elsewhere.

Topic catagories:

1 Rational use of energy
2 New and renewable sources of energy
3 Fossil fuels and clean fuel technologies
4 Environmental control and waste recycling
5 Energy policies and economics

The conference registration fee is USD 380 for active participants, if paid before 31 March 1996. Thereafter, the registration fee will be USD 450 for active participants. The reduced registration fee for students is USD 50.

For further information, please contact:

Mr Liu Feng/Mr Zhen Yingjun,
ENERGEX '96 Secretariat,
CICCST,
PO Box 9651,
Beijing 100086, China
Fax: (86 10) 257 5691

Conference Calendar

1996

Chemical physics for the 21st century

16–19 April
International Conference on Chemical Physics on the Border of the 21st Century. Moscow, Russia.
Prof. V. I. Goldanskii, Semenov Institute of Chemical Physics, Russian Academy of Sciences, Kosygin Street 4, Moscow 117977, Russia

Molecular order in polymers

21–24 May
2nd International Symposium on Molecular Order and Mobility in Polymer Systems. St. Petersburg, Russia.
Prof. T. M. Birshtein, Institute of Macromolecular Compounds, Russian Academy of Sciences, Bolshoy pr. 31, St. Petersburg, 199004 Russia

Free-radical polymerization

26–31 May
2nd International Symposium on Free-Radical Polymerization: Kinetics and Mechanism. Santa Margherita Ligure, Genoa, Italy.
Prof. S. Russo, Department of Chemistry, University of Sassari, Via Vienna 2, I-07100 Sassari, Italy. Tel.: +39 (79) 229556. Fax: +39 (79) 229559
Mycotoxins and phycotoxins

27–31 May
9th International Symposiums on Mycotoxins and Phycotoxins. Rome, Italy.
Dr Marina Miraglia, Instituto Superiore Sanità, Food Department, Viale Regina Elena, 299, I-00161 Rome, Italy. Tel.: +39 (6) 4990, ext. 377. Fax +39 (6) 4451767

Protein folding

17–20 June
International Symposium on Theoretical and Experimental Aspects of Protein Folding. San Luis City, Argentina.
Dr J. Vila, IMASL-Universidad Nacional de San Luis, Ejército de Los Andes 950, 5700 San Luis, Argentina

Oxidation of polymers

24–28 June
11th Conference on Polymers Thermal and Photo-induced Oxidation of Polymers and its Inhibition in the upcoming 21st Century. High Tatras, Slovak Republic.
Prof. L. Rychlá, Polymer Institute, Slovak Academy of Sciences, Dubravská cesta 9, 842 36 Bratislava, Slovak Republic

Surface forces

25–29 June
11th International Conference on Surface Forces. Moscow, Russia.
Dr L. B. Boinovich, Institute of Physical Chemistry, Leninsky Prospect 31, 117915, Moscow, Russia

Organic synthesis

30 June–4 July
11th International Conference on Organic Synthesis. Amsterdam, Netherlands.
Conference Secretariat ICOS – 11, PO Box 1558, 6501 BN Nijmegen, Netherlands. Tel.: +31 (80) 234471. Fax: +31 (80) 601159
Catalysis

30 June–5 July
11th International Congress on Catalysis. Baltimore, USA.
Prof. Gary L. Haller, Department of Chemical Engineering, Yale University, PO Box 208286, New Haven, CT 06520-8286, USA. Tel.: +1 (203) 432 4378. Fax: +1 (203) 432 4387

Organometallic chemistry

7–12 July
17th International Conference on Organometallic Chemistry. Brisbane, Australia.
17th International Conference on Organometallic Chemistry, Faculty of Science and Technology, Griffith University, Brisbane QLD 4111, Australia. Tel.: +61 (7) 38757217. Fax: +61 (7) 38757656. E-mail: icomc@sct.gu.edu.au

Chemical education

14–19 July
14th International Conference on Chemical Education—Chemistry: Expanding The Boundaries. Brisbane, Australia.
Dr W. Beasley, Graduate School of Education, The University of Queensland, Brisbane, Queensland 4072, Australia

Sweeteners

14–20 July
International Symposium on Sweeteners. Jerusalem, Israel.
International Symposium on Sweeteners, PO Box 50006, Tel.:- Aviv 61500, Israel. Tel.: +972 (3) 5140014. Fax: +972 (3) 5175674 or 5140077. E-mail: 100274.2665@CompuServe.COM

(Bio)degradable polymers

15–18 July
37th Microsymposium on Macromolecules (Bio)degradable Polymers: Chemical, Biological and Environmental Aspects. Prague, Czech Republic.
Dr B. Valter, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám 2, 162 06 Prague c-Petriny, Czech Republic

Carbohydrates

18th International Carbohydrate Symposium. Milan, Italy.
Prof. B. Casu, Istituto di Chimica é Biochimica 'G Ronzoni', via G. Colombo 81, 20133 Milan, Italy.
Photochemistry

21–26 July
16th Symposium on Photochemistry. Helsinki, Finland.
Prof. J. Wirz, Institut für Physikalische Chemie, Universität Basel, Klingelbergstr. 80, CH-4056 Basel, Switzerland

Solubility phenomena

22–25 July
7th International Symposium on Solubility Phenomena. Leoben, Austria.
Dr E. Königsberger, Symposium Secretary, Abteilung für Physikalische Chemie, Montanuniversität Leoben, A-8700 Leoben, Austria. Fax +43 (3842) 402308. E-mail: koenigsb@unileoben.ac.at

Macromolecules

4–9 August
36th International Symposium on Macromolecules. Seoul, Republic of Korea.
Dr Kwang Ung Kim, Secretariat of IUPACMACRO SEOUL'96, Division of Polymers, Korea Institute of Science & Technology, PO Box 131 Cheongryang, Seoul 130–650, Korea. Tel.: +82 (2) 957 6104. Fax: +82 (2) 957 6105. E-mail: iupac@kistmail.kist.re.kr

Excitonic processes

14–17 August
2nd International Conference on Excitonic Processes in Condensed Matter (EXCON '96). Bad

Schandau, Saxonia, Germany.
Prof. M. Schreiber, Faculty of Natural Sciences, Technische Universität Chemnitz-Zwickau, D-09107 Chemnitz, Germany

Coordination chemistry

18–23 August
31st International Conference on Coordination Chemistry. Vancouver, Canada.
31st ICCC Secretariat, UBC Conference Centre, 5961 Student Union Boulevard, Vancouver, BC, Canada V6T 2C9. Tel.: +1 (604) 822 1050. Fax: +1 (604) 822 1069

Macromolecular condensed state

20–25 August
International Symposium on Macromolecular Condensed State. Beijing, China.
Prof. X. Jin, Institute of Chemistry, Chinese Academy of Sciences, PO Box 2709, Beijing 100080, China. Tel.: +86 (1) 02564829. Fax: +86 (1) 02569564. E-mail: huangsl@rose.cnc.ac.cn

Physical organic chemistry

25–29 August
13th International Conference on Physical Organic Chemistry. Seoul, Republic of Korea.
Prof. J. Suh, Department of Chemistry, Seoul National University, Seoul 151–742, Republic of Korea. Tel.: +82 (2) 8862184. Fax: +82 (2) 8743704. E-mail: jhsuh@cd4680.snu.ac.kr

Biotechnology

25–30 August
10th International Biotechnology Symposium. Sydney, Australia.
10th IBS '96 Symposium Secretariat, GPO Box 128, Sydney, NSW 2001, Australia. Tel.: +61 (2) 2622277. Fax: +61 (2) 2622323. E-mail: veckels@tourhosts.com.au

Chemical thermodynamics

25–30 August
14th IUPAC Conference on Chemical Thermodynamics. Osaka, Japan.
Prof. M. Sorai, Executive Secretary of ICCT-96, Microcalorimetry Research Center, Faculty of Science, Osaka University, Toyonaka, Osaka 560, Japan. Tel.: +81 (6) 8505523. Fax: +81 (6) 8505526 (or 5288). E-mail:icct96@chem.sci.osaka-u.ac.jp

Environmental biotechnology

1–4 September
International Conference on Environmental Biotechnology. Palmerston North, New Zealand.
Conference Secretary, Environmental Biotechnology Conference, Process & Environmental Technology Department, Massey University, Palmerston North, New Zealand. Tel.: +64 (6) 3505351. Fax: +64 (6) 3505654.
E-mail: g.f.withers@massey.ac.nz

CHEMRAWN IX

1–6 September
Sustainable Production, Use, Disposal and Recycling of Materials. Seoul, Korea.
Organizing Committee & Secretariat, IUPAC CHEMRAWN IX, Tongwon B/D 6th Floor, 128–27 Tangju-dong, Chongno-ku, Seoul 110–071, Korea

Euroanalysis IX

1–7 September
Euroanaysis IX. Bologna, Italy.
Prof. L. Sabbatini, Dipartimento di Chimica, Università di Bari, Via Orabona 4, 70126 Bari, Italy. Tel.: +39 (80) 5442020/16/14. Fax: +39 (80) 5442026

Medicinal Chemistry

8–12 September
14th International Symposium on Medicinal Chemistry. Maastricht, Netherlands.
Prof. H. Timmerman, Department of Pharmacochemistry, Vrije Universiteit, De Boelelaan 1083, 1081 HV Amsterdam, Netherlands.

Food packinging

11–13 September
International symposium on Food Packaging: Ensuring Safety and Quality of Foods. Budapest, Hungary
Dr Laura Contor – ILSI Europe, Avenue E. Mounier, 83- Box 6, B-1200 Brussels, Belgium. Tel.: +32 (2) 7710014. Fax: +32 (2) 7620014

Characterization of porous solids

15–18 September
4th International Symposium on Characterization of Porous Solids (COPS-IV). Bath, UK
Elaine Wellingham, Conference Secretariat, Field End House, Bude Close, Nailsea, Bristol, BS19 2FQ, UK. Tel.: and Fax: +44 (1275) 853311

Chemistry of natural products

15–20 September
20th IUPAC Symposium on the Chemistry of Natural Products. Chicago, USA.
IUPAC Symposium Headquarters, 5999 Butterfield Road, Hillside, Chicago, Illinois 60161, USA

Multiphoton processes

30 September–4 October
7th International Conference on Multiphoton Processes. Garmisch Partenkirchen, Germany.
Prof. P. Lambropoulos, Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, D-85748 Garching, Germany

Step growth polymerization

End-September
International Symposium on Step Growth Polymerization, Related Processes and Materials. Paris, France.
Dr B. Sillion, Laboratoire de Chimie Macromoléculaire, Université Pierre et Marie Curie, 4 place Jussieu, 75252 Paris Cédex 05, France. Tel.: +33 (1) 78022078. Fax: +33 (1) 78022010

1997

Thermodynamics

5–8 January
International Symposium on Chemical and Biological Thermodynamics. Amritsar, India.
Prof. D. V. S. Jain, Department of Chemistry, Panjab University, Chandigarh 160014, India. Tel.: +91 (172) 541435. Fax: +91 (172 541409.
E-mail: dvs-jain@imtech ernet.in

Bioorganic chemistry

1–6 June
4th International Symposium on Bioorganic Chemistry. Biarritz, France.
Prof. A. Marquet, Université Paris URA CNRS 493, Laboratoire de Chimie Organique Biologique, Tour 44/45–4 Pl. Jussieu, 75252 Paris Cedex 05, France.

Recycling of polymers

14–17 July
38th Microsymposium on Macromolecules, Recycling of Polymers. Prague, Czech Republic.
Dr B. Valter, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám. 2, 162 06 Prague 6-Petriny, Czech Republic

Interfacial phenomena

21–24 July
17th Discussion Conference on Macromolecules surface and interfacial phenomena in Macromolecular Systems. Prague, Czech Republic.
Dr B. Valter, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám. 2, 162 06 Prague 6-Petriny, Czech Republic

Bioinorganic chemistry

27 July–1 August
8th International Conference on Bioinorganic Chemistry. Yokohama, Japan.
Prof. M. Hidai, Department of Chemistry & Biotechnology, Graduate School of Engineering, The University of Tokyo, Bunkyo-ku, Tokyo 113, Japan

IUPAC Congress

18–22 August
36th IUPAC Congress. Geneva,Switzerland.
Prof. J. Weber, Department of Physical Chemistry, University of Geneva, 30 quai Ernest-Ansermet, 1211 Geneva 4, Switzerland. Tel.: +41 (22) 7026111. Fax: +41 (22) 7026518. E-mail: weber@sc2a.unige.ch

IUPAC General Assembly

23–30 August
39th IUPAC General Assembly. Geneva, Switzerland.
The IUPAC General Assembly is not open for general participation but restricted to members of IUPAC bodies that meet on this occassion.

Coordination chemistry

24–29 August
32nd International Conference on Coordination Chemistry. Santiago, Chile
Prof. J. Costamagna, Departamento de Química, Facultad de Ciencia, Universidad de Santiago di Chile, Casilla 307, Santiago-2, Chile. Tel.: +56 (2) 6811644. Fax: +56 (2) 6812108. E-mail: jcostama@lauca.usach.cl

Spectroscopicum internationale

21–26 September
30th Colloquium Spectroscopicum Internationale 1997 (CSI). Melbourne, Australia.
The Meeting Planners, 108 Church Street, Hawthorn Victoria 3122, Australia. Tel.: +61 (3) 98193700. Fax: +61 (3) 98195978

1998

30 June–4 July
12th International Conference on Organic Synthesis. Venice, Italy.
Prof. C. Scolastico, Dip.to di Chimica Organica e Industriale, Università di Milano, Via G. Venezian 21, I-20133 Milano, Italy

Pesticide chemistry

2–7 August
9th International Congress on Pesticide Chemistry. London, UK.
Dr John F. Gibson, Secretary (Scientific), The Royal Society of Chemistry, Burlington House, London W1V OBN. Tel.: +44 (171) 4378656. Fax +44 (171) 7341227

Coordination chemistry

31 August–4 September
33rd International Conference on Coordination Chemistry. Florence, Italy.
Dr M. Perussini, ISSECC—CNR, Via Jacopo Nardi 39, 50132 Florence, Italy

2000

3–8 September
11th International Biotechnology Symposium. Berlin, Germany.
Prof. G. Kreysa, DECHEMA e.V., PO Box 15 01 04, D-60061 Frankfurt am Main, Germany

International Union of Pure and Applied Chemistry (IUPAC)

IUPAC

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The International Union of Pure and Applied Chemistry (IUPAC), formed in 1919, is a voluntary non-governmental, non-profit association of organizations, each of which represents the chemists of a member country.

Its objectives are:

- to promote continuing co-operation among the chemists of the member countries;
- to study topics of international importance to pure and applied chemistry which need regulation, standardization, or codification;
- to co-operate with other international organizations which deal with topics of a chemical nature;
- to contribute to the advancement of pure and applied chemistry in all its aspects.

The membership of IUPAC presently comprises 40 countries, each represented by a national organization, such as an academy of science or research council.

National Adhering Organizations

Academy of Scientific Research and Technology **(Arab Republic of Egypt)**
Asociación Química Argentina **(Argentina)**
Australian Academy of Science **(Australia)**
Ôsterreichische Akademie der Wissenschaften **(Austria)**
Nationaal Comité voor Scheikunde/Comité National de Chimie **(Belgium)**
Brazilian Chemistry Committee for IUPAC **(Brazil)**
National Research Council of Canada **(Canada)**
Sociedad Chilena de Química **(Chile)**
Chinese Chemical Society, Beijing and Chemical Society located in Taipei **(China)**
Croatian Chemical Society **(Croatia)**
Czech National Committee for Chemistry **(Czech Republic)**
Det Kongelige Danske Videnskabernes Selskab **(Denmark)**
Deutscher Zentralausschuss für Chemie **(Federal Republic of Germany)**
Suomen Kemian Seura **(Finland)**
Comité National Français de la Chimie **(France)**
Association of Greek Chemists **(Greece)**
Hungarian Academy of Sciences **(Hungary)**
Indian National Science Academy **(India)**
Royal Irish Academy **(Ireland)**
Israel Academy of Sciences and Humanities **(Israel)**
Consiglio Nazionale delle Ricerche **(Italy)**
Science Council of Japan **(Japan)**
Kuwait Chemical Society **(Kuwait)**
Koninkliijke Nederlandse Chemische Vereniging **(Netherlands)**
Royal Society of New Zealand **(New Zealand)**
Norsk Kjemisk Selskap **(Norway)**
Polska Akademia Nauk **(Poland)**
Sociedade Portuguesa de Quimica **(Portugal)**
Korean Chemical Society **(Republic of Korea)**
Foundation for Research Development **(Republic of South Africa)**
Russian Academy of Sciences **(Russia)**
King Adbulaziz City for Science and Technology **(Saudi Arabia)**
Slovak National Committee for Chemistry **(Slovakia)**
Slovenian Chemical Society **(Slovenia)**
Comisión Interministerial de Ciencias y Technología **(Spain)**
Svenska Nationalkommittén för Kemi **(Sweden)**
Neue Schweizerisches Chemische Gesellschaft **(Switzerland)**
Türkiye Kimya Dernegi **(Turkey)**
Royal Society **(United Kingdom)**
National Research Council, National Academy of Sciences **(USA)**

Chemistry International

IUPAC

1996, Vol. 18, No. 2 (March)

41 International Organization for Chemical Sciences Development (IOCD)

44 Transport properties of R134a

47 The IUPAC Solubility Data Project: Strategies and Coverage
J. W. Lorimer

50 News

51 ISO Standards

52 PAC Review

56 Commission and Committee News

61 Ultrafast chemistry with lasers

66 New publications

72 Affiliate Affairs

73 A Letter from Cuba
Alberto J. Nuñez Sellés

74 Conferences

77 Conference Calendar

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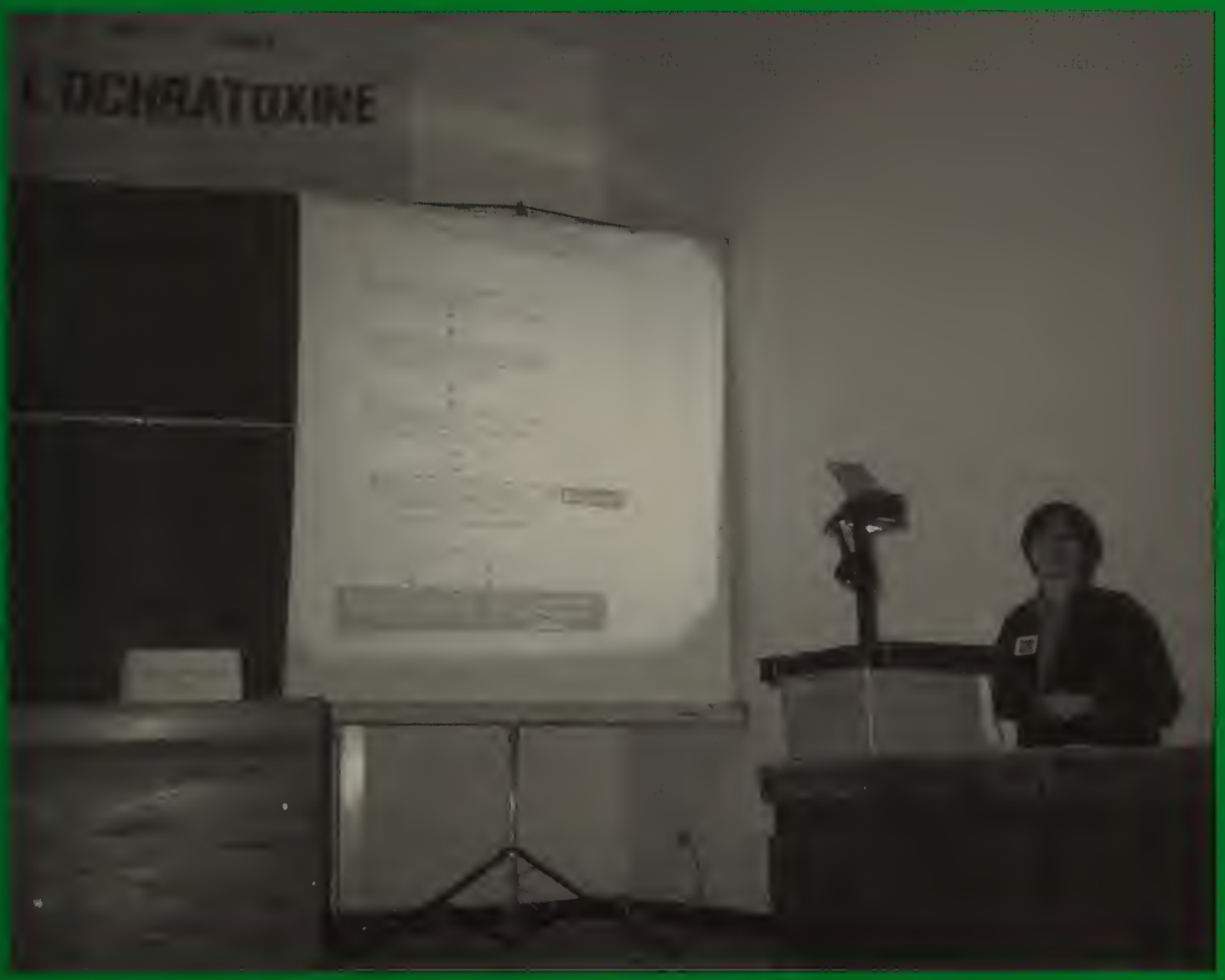

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1996, Vol. 18, No. 3 (May)

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Chemistry International

The news magazine of the International Union of Pure and Applied Chemistry (IUPAC)

EDITOR: Jeffrey H. Williams
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Front cover: Lecture at the recent IUPAC/UNESCO sponsored workshop on ochratoxins (Tunisia).

International Union of Pure and Applied Chemistry

Bohuslav Brauner's contributions to our knowledge of atomic weights

H. Steffen Peiser[a] and Jaroslav Kahovec[b]

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Who were the world's outstanding contributors to our knowledge of atomic weights? Most chemists would, with good cause, list some of the following: John Dalton, William Prout, Jöns Berzelius, Jean Stas, Frank Clarke, Theodore Richards, Wilhem Ostwald, Gregory Baxter, Otto Hönigschmid, Alfred Nier or Edward Wichers. Virtually no one would mention Bohuslav Brauner, who lived from 1855 to 1935, mostly in his native Prague. Some contemporary chemists may recognize his name. However, it is likely that this recognition is not for his atomic weight studies, but rather for other of Brauner's notable achievements which are well summarized in his biography[1] and may be listed as: (i) his resolution of problems with Mendeleev's periodic system; (ii) his clarification of the chemistry of rare-earth elements; (iii) his pioneering research on free fluorine; (iv) his establishment of the bivalency of beryllium; (v) his classical crystallographic investigations of morphology and isotropy, that is, cation, anion, or molecular substitution without discontinuous change of crystal cell geometry; (vi) his prolific authorship in chapters of Abegg's *Handbuch der anorganizchen Chemie*[2] on certain elements of the 1st, 2nd, 3rd, 4th, 5th and 7th groups of the periodic table, as then defined (that is, all except the 6th).

Biographies of Brauner have been published in Czech and English.[1,3] In 1877, as a 22-year-old student, Brauner wrote three papers: on the determination of arsenic as magnesium pyroarsenate, the determination of cobalt in potassium cobaltinitrate, and on fluorescence. He was inspired to work on fluorescence by Ernst Mach (1838–1916) who was at that time professor of physics in Prague. Mach is remembered for his studies of the motion of high-speed objects through gases, his philosophical ideas on science, and for his influence on Einstein. In the following year, Brauner completed his PhD research in Linnemann's organic chemical laboratory. The topic under investigation was the reaction of silver cyanate with isobutyl iodide. The formal award of the PhD degree (promulgation) was followed by his habilitation (*veniam docendi*) in 1889 on topics of rare-earth chemistry.

Brauner's expanding interests found inadequate outlet in Linnemann's laboratory, which was centered on organic chemistry. He therefore took advantage of opportunities to affiliate for one year to, firstly, Bunsen's renowned laboratory in Heidelberg (1878) and subsequently to Roscoe's group in Manchester (1880). It was during this time that Roscoe was President of the Chemical Society (London) and had began, with Schorlemmer, to write what became a well-known textbook: *A Treatise of Chemistry*. While in Manchester, Brauner lectured on his work on didymium (Di), which he showed to be a mixture of praseodymium and neodymium.

For the next 50 years, Brauner remained at the relatively disadvantaged Czech part of Charles University in Prague where, at first, the facilities were inadequate. Despite more attractive offers from abroad, he remained at Charles where he was promoted in steps to full professorship in 1897. He gradually won support for new buildings with improved equipment, and a steady stream of publications resulted.

In this article we focus on Brauner's atomic weight measurements, beginning with Be, undertaken before he was 23 years old. Later studies principally concerned: H, Be, C, N, F, Al, Si, Cl, Ar, As, Y, Ag, Sn, Sb, Te, I, La, Ce, Pr, Nd, Sm, Er, Hf, Bi, Th and U. He himself emphasized his atomic weight work in four papers: in 1888, 1889, 1897 and 1901, arguing persuasively for the use of the oxygen scale for atomic weight values. Many more elements combined with oxygen rather than with hydrogen, and the H/O mass ratio in water, which was at that time subject to larger uncertainty than the oxide ratios of most other elements, were also investigated. In these same papers, Brauner anticipated the modern view, adopted independently in 1969 by the Commission on Atomic Weights, CAW (recently renamed Commission on Atomic Weights and Isotopic

Bohuslav Brauner

Abundances—CAWIA) of the International Union of Pure and Applied Chemistry (IUPAC)[4] that uncertainty, derived from a careful analysis of the experimentally significant published data, had to be added to every atomic weight value. Brauner proposed, and adhered to, the following general rule for the publication of atomic weight values. When the uncertainty in the last digit exceeds 3, the value is abridged by removing the last digit to the nearest penultimate digit. In the authors' opinion, this rule has advantages over that adopted by the CAW prior to 1969.[4] As Brauner grew more confident in his own measurements, he ventured to express criticism of 'errors' in the international tables of atomic weights, [5]

In 1919, after the end of World War I, international scientific communications were re-established. IUPAC was established and accepted the responsibility for the International Commission on Atomic Weights, ICAW. In 1921, it reconstituted the Commission as the 'Committee on the Chemical Elements' (CCE) under the presidency of G. Urbain. IUPAC also included in this committee F. Clarke and T. Thorpe, and as new members: F. Aston, B. Brauner, A. Debierne, P. Guye, T. Richards and F. Soddy. Brauner, by virtue of his publications, was appointed chairman of the then informally constituted subcommittee on atomic weights. After the death of Guye, G. Baxter and A. Leduc were elected in 1922. In accord with the then current practice, the chairman, Brauner, was the principal author of the 1925 IUPAC Report. Although we have so far been unable to trace much of the relevant correspondence between Brauner and his subcommittee members, there is enough evidence in the CAWIA archives to prove that he diligently consulted with them.[6]

The Committee on the Chemical Elements was formally divided into three parts in 1930. One of these, the Atomic Weights Committee (AWC) under the chairmanship of Baxter, was responsible for the annual publication of atomic weight tables. Other members of the AWC were M. Curie, P. LeBeau, R. Meyer, and O. Hönigschmid. Brauner, then in his seventies, faded from view. Nevertheless, one of his innovative semantic proposals[7] has remained to the present, though it may be discouraged now by the International Organization for Standardization (ISO): 'atomic masses' (in contrast to 'atomic weights') refer only to individual isotopes. Much later, in 1947, Brauner's successor at Charles University, Professor Jindrich Krepelka, joined the Commission.

Brauner analysed atomic weight values in accordance with the principles he had earlier laid down. In 1922, he communicated to other members of the CAW his judgement on a large number of elements shown in the first column of Table 1. In chronological order, the table compares Clarke's previous 1920 values,[8] Brauner's 1922 values, the values in the CAW 1925 Report,[9] and the current IUPAC standard atomic-weight values.[10] Brauner's 1922 value for A_r(Bi), confirmed from his own handwriting, must surely be explained as a slip of his pen, since he explicitly refers to agreement with Hönigschmid's work (presumably ref.[11]), which proposes 209.0. This was disregarded by Clarke in 1920 in favour of the earlier, and erroneous, value of about 208.0. All told, Brauner must be given credit for major improvements in our knowledge of the atomic weights of Be, B, Si, Y, Sb, La and Bi.

One of Brauner's most outstanding atomic weight papers was co-authored by Krepelka,[12] and deals with the redetermination of A_r(Sn). Brauner's remarkably reliable estimation of uncertainties is also significant. Nevertheless, in the light of modern knowledge, he underestimated them for A_r(I) and, to a lesser extent, for A_r(Br), the latter affecting the all-important A_r(Ag) value. That remained in error by 8 parts in 10^5, contrasted with Brauner's own estimate of 5 parts in 10^5, but still a remarkable achievement for a chemical determination at that time.

Atomic weights, the Mendeleev periodic table, radioactivity, isotropy and the optimum scale for the atomic weights were the key issues in inorganic chemistry at Brauner's time, and he contributed significantly to all of these topics. He combined experimental chemical expertise with skills comparable to those of Richards, Hönigschmid and Baxter. In the analysis of published

Table 1 Atomic weights of some elements*

Element	Clarke (1920)	Brauner (1922)	CAW[9] (1925)	CAWIA[10] (1993)
Be	9.093	9.02 ++	9.02	9.012182 (3)
B	10.912	10.91	10.82 ++	10.811 (5)
C	12.003	12.005	12.000 –	12.011 (1)
N	14.008	14.006	14.006	14.00674 (7)
F	19.011	19.00 +	19.00	18.9984032 (9)
Al	27.039	27.0 +	26.97 +	26.981539 (5)
Si	28.255	28.11 ++	28.06 –	28.0955 (3)
Cl	35.460	35.453 +	35.457 –	35.4527 (9)
Y	89.33	89.33	88.9 ++	88.90585 (2)
Ag	107.88	107.876 +	107.880 –	107.8682 (2)
Sn	118.71	118.70 –	118.70	118.710 (7)
Sb	120.06	121.77 ++	121.77	121.760 (1)
Te	127.53	127.61	127.5 –	127.60 (3)
I	126.93	126.927 +	126.932 –	126.90447 (3)
La	138.80	138.92 ++	138.90 +	138.9055 (2)
Ce	140.21	140.22 –	140.25 –	140.115 (4)
Pr	140.88	140.95 –	140.92 +	140.90765 (3)
Nd	144.24	144.3 –	144.27 +	144.24 (3)
Sm	150.40	150.4	150.4	150.36 (3)
Bi	208.06	209.9	209.00 ++	208.98037 (3)
U	238.15	238.2 +	238.17 +	238.0289 (1)

* The values are scaled to A_r(O) = 16 exactly, the values in the last column are concordant with A_r(O) = 15.9994. The uncertainties are given in parentheses, following the last significant figure to which they are attributed.
++ considerably superior, + slightly superior, – inferior to prior value.

literature he seems to have bettered the famed achievements of Clarke.[8]

Why then, we must ask ourselves, has he been almost forgotten? One reason may have been that he was a native of a small country, which is a handicap for any scientist; but Prague at that time was certainly not a scientific backwater. In addition, Brauner appears to have had some bitter enemies, but he was willing, and able to defend himself, showing, for example,[13] that a 'Herr Jones' had not demonstrated any right to criticize Brauner's A_r(La). In the controversy on didymium, Brauner seems to have been recognized as the injured party. One must also remember that long-term memorials in history can only be accorded to very few scientists. In atomic weight determinations Brauner deserves to be remembered as one of the leaders of chemistry of the early part of the 20th century.

Acknowledgements

We are much indebted to Dr O.T. Benfey, of the Chemical Heritage Foundation and Mr W.G. Leight, of the National Institute of Standards and Technology, for reading the manuscript and making many valuable suggestions which we have gladly adopted. We also gratefully acknowledge the continuing encouragement of Dr T.B. Coplen, currently the Secretary of the IUPAC Commission for Atomic Weights and Isotopic Abundances.

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Letters to the Editor

Ethics in modern science—a framework for discussion

Joshua Jortner

Introduction

Science is unique amongst human endeavours in that its entire edifice, and continued advance, rests on the honesty and the personal integrity of its practitioners, scientists. It is a collective effort in which each individual scientist can, hopefully, depend on the truthfulness of other scientists.

Ethical guidelines of conduct for scientists have existed for as long as the scientific enterprise. Due to direct public exposure, this is particularly the case in the bio-medical field. In the past, these guidelines were largely unwritten, but the rapid growth of science, and the increase in the number of scientists this century has perhaps created a need for renewed discussion and more explicit formulation of the problem of ethical standards in science.

(*Chemistry International*, September 1995, page 161)

In the September 1995 issue of *Chemistry International* (*CI*) Prof. Joshua Jortner, President of the Israel Academy of Sciences and the Humanities and, since 1 January 1996, Vice-President of IUPAC, published an article entitled *Ethics in Modern Science—a Framework for Discussion.* Prof. Jortner's article was followed in that issue of *CI* by one written by the Editor entitled *The Scientist and Ethics: Cautionary Tales.* The idea behind the first of these two contributions was to formulate a code of ethics for scientists. The second of these two

articles pointed out what can happen when scientists ignore or disregard ethical issues in their work.

Comments on these articles were invited and we give below three such comments which have been received at this office.

SIR: I read with some interest Joshua Jortner's article and your 'Cautionary tales' on ethics in science, in the September *Chemistry International*. I think that the matter of ethics in science is important and has received too little attention in the past. So I applaud your raising the consciousness on these issues.

In neither Jortner's or your articles did I find a discussion of the obligation of the scientist to make available the data on which a publication is based. My question: do you consider this an ethical issue? Are there guidelines that you are aware of that deal with these obligations, with attendant issues regarding publication of work by the receiving scientist that makes use of the data supplied on request.

Imagine a scenario in which scientist A publishes a paper that reaches a certain conclusion. Scientist B requests the original data to allow him/her to conduct his/her own independent examination to extend the analysis by A or to employ different types of data analysis. scientist A senses/fears that scientist B may reach a different conclusion, that might or might appear to discredit the original work. Can scientist A ethically withhold the data, perhaps claiming that he/she intends to write a further paper with these data and doesn't want to turn the data over to B until such time. Of course it might take a while to write the paper; then of course the paper has to be reviewed, etc. Perhaps there will be yet another paper that A wants to write, so he/she is still not ready to hand over the data. At what point, if ever, is A obliged to release the data? And to whom?

I should appreciate any pointers you can call my attention to that address this issue and of course any thoughts you might have on the matter.

Thank you.

Stephen E. Schwartz
21 September 1995

Environmental Chemistry Division, Brookhaven National Laboratory, Upton, NY, USA

Some marginal problems of scientific ethics

SIR: Professor Joshua Jortner's fine discussion of ethics in modern science (*Chemistry International*, September 1995) gives attention to the ever-important matter of scientific integrity.

Discussions of scientific ethics define certain practices as clearly unethical. Others however, are borderline. I now mention some of the latter. My aim is to provoke thought and discussion.

Sloppy work and/or records. A clinical researcher who was careless about sterilizing hypodermic needles while administering a new drug by injection to 60 volunteer tuberculosis patients would be condemned as unethical. Laymen would see that a dirty needle might introduce a pathogen, causing a serious infection. Scientists would share that concern, but also would perceive that such an infection would confound the experiment.

Perhaps publication of sloppy chemical laboratory work should also be judged unethical, unless its description informs a reader (in effect) that the experiments were sloppy. (There is a place for the 'quick and dirty' experiment, if reported as such.) One can argue that use of dirty glassware, defective meters, reagents of unverified identity or purity, spills during transfers, careless reading of instruments, and/or mistakes in calculation would generally disqualify an experimental result. If a sloppy experiment is reported as though conducted carefully, a possibly erroneous result in the chemical literature may obstruct scientific progress. It may cause others years of extra work before they conclude that a certain report must be wrong.

Failure properly to label samples generated in experimental work is arguably an aspect of sloppiness. A worker may painstakingly prepare, isolate and purify several materials, put them carefully in little beakers covered by watch glasses, but neglect to label them, being sure that the beaker in the back left corner of the lab bench contains compound A, the beaker at the right end of the shelf compound B, etc. Why bother to write out labels when one knows so well the contents of each beaker? But if the worker suddenly got influenza, were away from the laboratory for two weeks, upon return was only fairly sure which compound was which, but nevertheless proceeded to use the materials in further experiments relying on such recollections, would that constitute sloppy work? A wrong recollection might cause a wrong report to appear in the literature.

Sloppiness in records of laboratory work is similar. If manipulations and observations were not carefully recorded in a notebook, or spectral charts and the like were not definitively labelled, the scientist in writing a report or a manuscript might depend on memory to make connections or supply details not present in the written record. Human memory is notoriously fickle, again a wrong result may appear in the literature.

In such cases, a scientist completely honest in intent might report a wrong result due to sloppiness. The disservice to science is as bad as if a wrong report stemmed from fraud.

Selective reporting of observations. If a clinical researcher, working meticulously, found that the health of 32 of 60 tuberculosis patients were significantly improved by administration of a new drug, while 28 showed no improvement, and reported the improvement of the 32 without mention of the 28, that would

clearly be unethical. Do some of the publication practices of chemists approach such behaviour? For example, a synthetic chemist who tries eight ways to convert compound C into D, of which one is successful and seven are not despite careful work, and reports only the success without mention of the failures. How about a physical organic chemist who plotted eight quantitative observations against some theoretical parameter, found seven points to be in good linear array but one to be an 'outlier', and published the seven without the 'outlier'? (Incidentally, is that chemist engaged in self-deception?) We will all agree, however, that discarding the result of an experiment *known* to be faulty, owing say to a spill during quantitative transfer or malfunction of an instrument, is legitimate.

Maybe we should also question the way some organic chemists report elemental analyses. Analysis of a carefully purified substance may yield percentages of carbon and hydrogen not sufficiently close to theoretical to satisfy the chemist's standards. If the substance is then repurified, re-analysed, the resulting percentages may be close enough to satisfy the chemist. If the latter analyses but not the former are reported, is that also deceptive both to others and to self? Unless there were evidence that the second sample really were more pure than the first, reporting only the latter analysis amounts to choosing to publish the data that please the chemist.

Selective reinvestigation. Scientists seek order in the natural world. A scientist who finds numerous observations to fall into a pattern, while a few don't fit, may re-examine the nonconforming reports to see whether they were erroneous. Experiments may be repeated, calculations checked, observations of natural phenomena (e.g. eclipses of the sun) compared with others of the same phenomenon. If the early report were judged to be mistaken, it may be either omitted from publication or replaced by a recalculated or redetermined result. So far so good. In view of the possibility that some observations that fell into accord with the generalization may also have been faulty, should the scientist undertake to scrutinize them with equal thoroughness? If he/she does not, is the scientist unethical by setting a lower standard to acceptance of pleasing as compared to unwelcome data?

It would be useful if others would identify practices in science that are at or just beyond the boundary of ethical behaviour.

Joseph F. Bunnett
6 October 1995

University of California, Santa Cruz, CA, USA

SIR: I have been very interested by the paper of Prof. Jortner on ethics in modern science and share generally the views expressed therein. Nevertheless, I would like to raise two points.

I am not convinced about a 'diminished esteem for academic research' as stated on page 161, *Chemistry International*, September 1994. Actually a rather recent survey by CEFIC shows that the credibility of scientists and university professors is quite high in the public mind, at least for what regards environmental questions. What puzzles the public is not 'publicity about fraud in science' but rather divergences in publicly expressed specialists' opinions. People with limited scientific literacy tend to believe that scientists hold 'the truth' and have some difficulties to make the difference between observed facts and their varying interpretations.

The use of scientific jargon in public communications doesn't help to make science better understood by the general public. Therefore, I share totally the views of the author on the importance of 'inspiring public confidence in science' and of 'anything which will increase the scientific literacy of the general public', especially good and relevant teaching of sciences in secondary education.

My second comment refers to ethical 'normative rules'. From my understanding, the author seems to limit ethics essentially to basic research. This is supported by statements on 'communalism, openness and information sharing', 'publication in scientific journals'.

As a member of the Committee on Chemistry and Industry of IUPAC, I would like to react by saying that apart from these criteria, ethical rules apply also to scientists in industry. Even if there are obviously different rules governing the propriety and the diffusion of scientific information in academic, industrial or military research 'accurate scientific reporting must adhere to the norms of objectivity, honesty, precision and recognition of priority' applies for all scientists.

Therefore, I would suggest that 'rules of publication' should be revised to take both 'private' and 'public' research into consideration, even if I adhere to those rules as worded in the paper for what regards 'public' research.

Sincerely yours,

Prof. G.J. Martens
9 October 1995

SOLVAY S.A., Bruxelles, Belgium

IUPAC Colleagues deceased

Denmark: Dr J. B. Jensen (20 October 1995) Commission on Solubility Data (1983–1995)

Russia: Prof. L. V. Gurvich (23 August 1995) Physical Chemistry division Commtitee (1973–1977), Commission on Thermodynamics (1967–1977), Commission on High Temperature and Solid State Chemistry (1997–1989)

IUPAC–UNESCO collaboration

Recently, IUPAC has been collaborating with the United Nations' Educational, Scientific and Cultural Organization (UNESCO) to participate in chemistry projects that are of mutual interest. More precisely, to undertake in close cooperation with UNESCO programmes in chemistry for the needs of the least developed countries. Such programmes include: training courses, workshops, visits and lectures by expert chemists, training of technicians, and provision of chemistry texts, in particular those of IUPAC, to reseachers, teachers and students in developing countries.

Here we report on such a programme which has recently come to an end. As part of IUPAC's work of assisting chemists in least developed countries, two worshops were organized by scientists from the Food Chemistry Commission of the old Applied Chemistry Division, now restructured as the Division of Chemistry and the Environment, and a third project involved the Clinical Chemistry Section of the new Division of Chemistry and Human Health.

International IUPAC/UNESCO Workshop on Ochratoxin (14–17 November, 1995)

Introduction

Ochratoxin A (OTA), a potent nephrotoxic, carcinogenic and hepatotoxic mycotoxin produced by several fungal species, can contaminate human foods and animal feeds as a result of the currently unavoidable invasion by molds during improper storage of the food stuff. The need to limit OTA in foods/feeds is based on two major concerns: (a) the adverse effects of OTA-contaminated foods/feeds on human and animal health; and (b) the presence of OTA residues or toxic metabolites in animal tissues used as human foods, such as pork and poultry products. In the Balkans (Bulgaria, Romania and ex-Yugoslavia), ochratoxin contamination has been implicated in a human disease known as Balkan Endemic Nephropathy (BEN). BEN is characterized by high incidences of end stage renal failure and/or tumours of the urinary tract. Recent studies have reported similar disease symptoms and ochratoxin metabolites in blood from patients in Tunisia and Algeria.

The present workshop was conducted at the School of Medecine of the University of Sousse, Tunisia, and provided a training program of on-site personnel for the establishment of a food safety program for ochratoxin. Dr J. Marc Fremy (Centre National d'Etudes Vétérinaires et Alimentaires, Paris, France), and Prof. Douglas L. Park (Louisiana State University, Baton Rouge, USA), both members of IUPAC's Division of Chemistry and Environment (Commission on Food Chemistry, VI.5), were the IUPAC contacts. Funding for the project was provided mainly by IUPAC/ICSU/UNESCO, with additional support offered by FAO (Roma, Italy), the Association Africaine de Microbiologie et d'Hygiene Alimentaire (AAMHA, Sousse, Tunisia), CNEVA (Paris, France), LSU (Baton Rouge, USA), and the International Agency for Research on Cancer (IARC/WHO, Lyon, France). Support from Rhône Poulenc Diagnostic (Lyon, France) was also provided by furnishing immunochemical test kits and by participating in the teaching faculty.

The local organization was undertaken by Prof. Mongi Jemmali and Prof. Salem Said in a very friendly atmosphere. Lectures, Laboratory training sessions were held in university facilities. A scientific Committee composed of Prof. D.L. Park (LSU), Prof. M. Jemmali (AAMAH), Dr J.J. Castegnaro (IARC/WHO), Dr C. Canet (FAO) and Dr J.M. Fremy (CNEVA, Chair) organized the Workshop through meetings in Paris (France) and correspondance over the 8 months prior to the Workshop. Internationally recognized experts on Mycotoxins were selected for the teaching faculty and the selection of attendees was based on their science background and the possibility of training other analysts in their respective organizations and/or countries.

Fifteen participants from seven countries attended the workshop: Tunisia (9), Egypt (1), Ivory Coast (1), Morocco (1), Congo (1), Guinea Bissau (1) and Senegal (1). The training programme provided information through a series of lectures on: fungal growth and OTA

Fig. 1 Teaching at the International IUPAC/UNESCO Workshop on Ochratoxins, School of Medicine of the University of Sousse, Tunisia, 14–17 November 1995.

Fig. 2 Laboratory classes at the International IUPAC/ UNESCO Workshop on Ochratoxins, School of Medicine of the University of Sousse, Tunisia, 14–17 November 1995.

production in cereal grain, occurrence of OTA in plant and animal products, preventive measures, toxicity and metabolism of OTA, a review of analytical methods, sampling procedures, regulatory limits, decontamination protocols, good laboratory quality assurance, and international programmes. 'Hands on' laboratory training for specific analytical procedures applicable to products of affected regions was also provided.

Specific analytical procedures studied included: immunochemical method test kit for OTA detection, TLC method with physicochemical clean-up for OTA determination in cereals, HPLC and TLC method with immunoaffinity chromatography clean-up for OTA determination in cereals, and animal tissues, as well as HPLC procedure for OTA residue determination in blood. At the end of the workshop, guidance and recommandations for the establishment of a monitoring programme and preventing measures were set. In the laboratory portion of the training, the students were able to detect OTA in wheat contaminated at 10 and 50 µg/kg, in animal serum spiked at 10 ng/mL, and in poultry liver spiked at 10 ng/g. A document including the analytical method protocols was distributed to the attendees.

Recommendations formulated during the Workshop

Sampling: (i) Conduct studies to determine appropriate parameters for sampling plans for ochratoxin contamination in various matrices, i.e. animal feed, human foods and biological materials. Such sampling plans must include sample collection methods, preparation of samples for analysis, and analytical to include. (ii) In the absence of acceptable sampling plans use those developed for aflatoxin and other mycotoxins as a guide.

Monitoring Programmes: Develop a food safety monitoring programme for ochratoxin including: (i) monitoring the formation of ochratoxin in raw commodities, (ii) determination of ochratoxin and/or metabolites in foods derived from animal sources, (iii) establishment of recommended control measures, (iv) development of decontamination programmes/procedures, and (v) the establishment of procedures for handling violative product.

Laboratory Quality Assurance: (i) Utilize, where feasilble, analytical methods that have stood the rigours of interlaboratory validation studies to determine precision and accuracy parameters. (ii) Follow, where available, laboratory check–sample programmes for mycotoxins. (iii) Follow sound laboratory practice for record keeping, calibrations and standards, calculations and procedures.

Determination: Explore physical, chemical and biological methods of reducing risks posed by ochratoxin contanimation.

Prevention: Follow sound agricultural procedures for crop production, insect control, harvesting, storage, transpiration and treatment for commodities susceptible to mould growth and mycotoxin formation. Procedures may include limited insect infection in the field, lowering moisture levels during storage, and developing decontamination procedures for ochratoxins.

A diploma attesting the participation in this workshop was distributed to each participant. Further contacts and assistance to the participants will be provided for the application of these measures.

International IUPAC/UNESCO Workshop on Ciguatera (8–10 November, 1995)

Introduction

Ciguatera fish poisoning is a serious illness manifested in humans by a variety of neurotoxic, gastrointestinal, and cardiovascular symptoms. It results from the consumption of certain tropical and subtropical fishes (up to 400 species) which have accumulated toxins produced by microscopic algae, i.e. dinoflagellates. Ciguatera toxins are odorless, tasteless and generally undetectable by any simple chemical test. The number of cases of ciguatera fish poisoning occurring each year has been estimated to be as high as 500 000. Although ciguatera fish poisoning occurs primarily in tropical regions of the world, outbreaks have been reported in continental US and Canada due to inter-regional shipments of seafood.

Because of the severity of the illness, public health agencies strive to implement a seafood safety programme. Programmes that are designed to provide assurances that foods susceptible to natural toxin contamination are safe to eat require several facets, including the market-place screening of suspect foods, separation of adulterated product to lower risk uses, and, where feasible, the development of monitoring programmes to predict potentially hazardous food pro-

duction/harvesting areas.

Public health research activities with respect to phycotoxin contamination, i.e. ciguatera, have focused on the protection of human health and the enhancement of commerce from subtropical reef fish. This goal can only be realized, however, by having a control programme for effectively removing contaminated fish from the market-place. In order to understand how to set up an effective seafood safety monitoring programme, it is necessary to understand how the product becomes toxic and to have the analytical tools to identify high-risk products. Quick and reliable analytical assays are crucial for the effective monitoring of seafood safety programmes. Historically, assays for the analysis for ciguatoxins have been time-consuming and lacked specificity. The solid-phase immunobead assay (S-PIA) has the highest potential for application to the market-place screening of fish products for ciguatera toxicity. Testing fish early is recommended, since this will minimize the product cost and potential economic losses to industry. The S-PIA kit can be used on-board fishing vessels, at receiving docks, processing plants, distribution organizations, retail outlets, consumers and regulatory agencies.

A key aspect of an effective seafood safety monitoring programme, where feasible, is the establishment of a programme for predicting and identifying high-risk fishing areas. This can be accomplished through the testing of marine specimens endemic to fish harvesting locations. This will vary for ciguatera fish poisoning or diarrhoeic shellfish poisoning (DSP). Since seafood commonly associated with ciguatera poisoning outbreaks come from highly mobile fish, the collection and testing of fish alone could provide incorrect information, giving both false positive and false negative predictions. This potential problem can be corrected by identifying and testing a specimen or biomarker of limited motility, for example, invertebrates endemic to the fishing area.

As an example of such correlations, the Ciguatect™ solid-phase immunobead assay was used to screen 36 species of near-shore invertebrates off the coast of the Island of Hawaii for ciguatoxin and related polyether compounds. Specimens included snails, sea urchins, sea cucumbers, crabs, briale stars, bivalves, and zoanthids. Invertebrates were collected at six 'toxic' locations with a documented history of ciguatera fish poisoning, and at three 'nontoxic' sites where there had been only one reported case of ciguatera since 1980.

A significant positive correlation between the assay results and site-specific ciguatera history was found for the cowry *Cypraea maculifera*. While assay results for most other species indicated very low or no ciguatoxin present, cone snails (*Conus* sp.), ophiuroids (*Ophiosoma* sp.), and sea cucumbers (*Holothuria* sp.) frequently tested positive. There was no correlation, however, for these three genera between assay results and site history. The results suggest that invertebrates, particularly grazers and deposit feeders—especially cowries—accumulate ciguatoxins and related polyether compounds at sites known for ciguatera fish poisoning outbreaks, and have the potential utility of being bio-indicators of reef toxicity. This marine species, or another invertebrate native to the area under study, could become an integral part of a ciguatera monitoring programme.

The S-PIA has been used to test for DSP toxicity potential in mussels implicated in a DSP outbreak in Denmark and in DSP depuration monitoring studies along the Atlantic coastline of France. The study results demonstrate that the assay can identify DSP-contaminated shellfish and serve as a useful tool for monitoring shellfish on-shore or during depuration operations to determine when shellfish can enter the market following certain dinoflagellate blooms.

Scope of the Workshop

The workshop provided a training programme of on-site personnel for the establishment of a seafood safety programme for ciguatera fish poisoning.

The present workshop on ciguatera, held in the Dominican Republic, focused on providing information and training to professional scientists and public health administrators responsible for aquatic biotoxins so that they could utilize this knowledge in their respective organizations and establish preventive control and monitoring programmes for ciguatera fish poisoning. The lecture sessions included information and direction on: (i) the diseases associated with foodborne toxins and micro-organisms; (ii) the incidence and occurrence of ciguatera fish poisoning; (iii) chemical characteristics and structure of aquatic biotoxins associated with ciguatera; (iv) micro-organisms such as dinoflagellates responsible for toxin production in the ocean environment, and fish species reported to be associated with ciguatera fish poisoning; (v) symptoms expressed and

Fig. 3 Participants at the International IUPAC/UNESCO Workshop on Ciguatera, Santo Domingo, Dominican Republic, 8–10 November 1995.

inherent with the poisoning event in humans and treatment procedures; and (vi) laboratory training.

Such laboratory training included: (i) dinoflagellate collection and identification procedures; (ii) toxicity testing assays, such as the mouse bioassay (utilizing intraperitoneal injections of toxins and fish extracts), and the brine shrimp (*Artemia* sp.) assay; and (iii) the innovative immunobead assay (S-PIA, Ciguatect™, HawaiiChemtect International, Pasadena, CA). These procedures were demonstrated and applied to the determination of ciguatoxin and related toxins directly on fish tissue or extracts. Fish samples and extracts associated with ciguatera fish poisoning cases in the Dominican Republic were tested with these procedures. Ciguatoxicity as well as the presence of ciguatoxin and ciguatera-related toxins, including okadaic acid, were confirmed.

Fifteen research scientists and officials representing 10 health and regulatory agencies, and industry from the Dominican Republic participated in the workshop. These regulatory authorities included: Centro de Investigaciones de Biologia Marina (CIBIMA/UASD), Instituto Dominicano de Tecnologia Industrial (INDOTEC), Secretaria de Estado de Agricultura, Secretaria de Estado de Industria y Comercio, Secretaria de Estado de Salud Publica, Laboratorio Nacional de Salud Publica, SESPAS, Laboratorios Nacional, and Laboratorios Veterinarios Central.

One participant from INDOTEC and one from the Dominican Republic Department of Health will receive further training at Louisiana State University, Baton Rouge, Louisiana. Internationally recognized experts in various aspects of ciguatera fish poisoning representing the University of Southern California, Louisiana State University, the University of Miami, Centre National d'Etudes Vétérinaires et Alimentaires (CNEVA), the Cuban Department of Health, and the Pan American Health Organization (PAHO/WHO) comprised the faculty.

Dr Douglas L. Park, Department of Food Science, Louisiana State University, Baton Rouge, Louisiana, USA, and Dr Jean Marc Fremy, CNEVA, French Ministry of Agriculture and Fisheries, Paris, France organized and coordinated the workshop activities.

Quality Improvement Programme for Clinical Chemistry Laboratories in Kenya (14–15 August 1995)

Introduction

Appropriate laboratory services form an integral part of any health care delivery system. In order to assist in the accurate diagnosis of a patients' diseases, a laboratory must be able to produce consistent analytical results. Fortunately, many countries have mechanisms to ensure that quality assurance programmes are used in all clinical laboratories.

In Kenya, the local use of quality control and quality assurance schemes has been inconsistent. The Clinical Chemists Association of Kenya (CCAK) has, over many years, held seminars and workshops aimed at creating an awareness for the necessity of having quality control schemes as part of good laboratory practice.

The Kenyan Ministry of Health recently emphasized its mission to ensure quality health care for all Kenyans. This cannot be achieved, however, without having a quality laboratory service. The present initiative of the CCAK is therefore timely in relation to the Ministry of Health's concerns.

The present initiative represents an extension of a programme begun under the auspices of the International Union of Pure and Applied Chemistry and the International Federation of Clinical Chemistry (IFCC) which supported a quality assurance workshop in Nairobi in January 1993 funded through the International Council of Scientific Unions (ICSU). The current programme was funded jointly by UNESCO and the Royal Society of Great Britain.

The purpose of this programme was to establish a workshop of invited senior laboratory workers in Kenya committed to quality assurance, at which the problems of establishing a permanent internal control and external assessment programme could be discussed with the international visiting team, and that from this workshop recommendations would be made and presented to the Ministry of Health. To achieve these ends, three criteria had to be met: the participants from within Kenya must be committed to quality assurance; must be sufficiently senior to be able to influence future policy, and must represent the relevant interested groups namely, public and private hospitals, mission hospitals, the universities, and government (through the Public Health Department).

The international team must be similarly committed to quality assurance and experienced in the problems of establishing internal and external programmes. For these reasons, the Chairman of the Australian Quality Assurance Programme of the Royal College of Pathologists of Australasia and Australian Association of Clinical Biochemists (RCPA-AACB) was invited to participate, and was supported by RCPA-AACB. Similarly, representation from Randox Laboratories Limited who organize an international commercial quality assurance programme was also invited.

Workshop – Quality Assurance in the Practice of Clinical Chemistry: Proposals and Recommendations

The following aims, objectives and strategic plan for a quality improvement programme have been developed

for clinical chemistry laboratories in Kenya. They are drawn from the proceedings and discussion of the Workshop on Quality Assurance conducted in Nairobi on the 13th and 14th of August 1995. They also represent the unanimous views of those present.

Specific objectives

To improve the quality of laboratory practice by:

(i) Providing appropriate educational programmes in good laboratory practice.
(ii) Implementing an appropriate internal quality control programme in all clinical chemistry laboratories in Kenya
(iii) Establishing and implementing an external quality assessment programme suitable for Kenyan laboratories.
(iv) Establishing a mechanism for ensuring continuity of internal and external quality programmes.
(v) Establishing a mechanism for laboratories to maintain acceptable standards of performance.

Strategic plan

(i) To obtain approval and support from the Ministry of Health for the programme.
(ii) To establish a Steering Group for the quality improvement programme.
(iii) The Steering Group shall consist of representatives from the following:
  (a) Clinical Chemists Association of Kenya
  (b) Ministry of Health and National Public Health Laboratory Services
  (c) Kenyatta National Hospital
  (d) University of Nairobi
  (e) Private Hospitals

Meeting with Dr P.O. Chuke, World Health Organization

Prof. Orinda (Chairman of the Clinical Chemists Association of Kenya (CCAK)), Dr Kiaira, Mr Geary, Mr Russell, Dr Wyndham and Dr Worth met with Dr Chuke, the WHO representative in Kenya.

Professor Orinda gave a summary of the progress of the workshop, and the outcome of its discussion. He explained that a draft paper of recommendations had been prepared and communicated their contents to Dr Chuke. Dr Wyndham gave a brief explanation of the Australian External Quality Assessment programme, its aims, and how these have been achieved.

There followed a general discussion in which the importance of total quality management in laboratories was emphasized and how it is essential to the overall quality of patient care, and how poorly resourced laboratories are a false economy if these quality standards cannot be achieved. These views were well recognized by Dr Chuke and he pledged the support of the WHO to the establishment of quality assessment programmes in Kenya.

Prof. Orinda raised the issue of the organization and monitoring of external assessment programmes, and mentioned the concept of a steering group representing the interested parties, as indicated in the draft recommendations. Again, this principle would meet with the support of the WHO. It was also pointed out that the workshop had been fortunate in receiving the support of Randox Laboratories and that Prof. Orinda would be having further discussions with Mr Russell concerning the possibility of establishing a commercially based programme targeted, in the first instance, at a small group of laboratories.

Dr Chuke agreed to raise these matters with the Regional Office of the WHO in Brazaville with the view of seeking their support. It was recognized that applications for financial support for a defined programme would have to have the support of the Ministry of Health, indeed, application would have to be made through the Ministry.

Meeting with Dr Gesami, Ministry of Health

Prof. Orinda and Dr Worth met with Dr Gesami, the Deputy Director of Medical Services at the Ministry of Health, who opened the workshop programme on Monday 14 August 1995.

Dr Gesami recognized the importance of this programme and its aims, and also the way in which it fitted in with the Ministry's present initiative on quality issues.

The problem, however, is one of resourcing—funding is limited and programmes have to be prioritized. For this reason it was important that Prof. Orinda and Dr Worth were able to meet with Dr Gesami. Prof. Orinda presented Dr Gesarni with a draft of the recommendations agreed by the workshop. Dr Gesami thanked Prof. Orinda and expressed his appreciation of the efforts of the workshop, giving his assurance that the recommendations would receive his support and that he would refer the matter to the Director of Medical Services.

Conclusions

The two-day workshop on quality assurance in the practice of clinical chemistry provided an ideal forum for the presentation of practical advice in the establishment of internal control and external assessment programmes. It provided a useful mix of approaches, namely, by clinical chemists from the Royal College of Pathologists of the Australasia/Australian Association of Clinical Biochemists Quality Assurance Programme, and from Randox International Quality Assurance Scheme. Attention was drawn to a draft IFCC document, 'Improving Analytical Quality in Developing Countries by Establishing and Managing External Quality Assessment Schemes', prepared for the Committee on Analytical Quality of the IFCC Education and Management Division, by P. Hill, A. Uldall and P. Wilding. A check list of questions that need to be con-

sidered before implementing an external quality assurance scheme was presented in tabular form.

Participants for this workshop were selected for their enthusiasm and commitment to quality management, and also in order to represent the various interested factions within laboratory health care in Kenya. Consequently, there was free-flowing and lively discussion throughout the workshop. This in turn resulted in the proposals and recommendations which have the unanimous support of the workshop participants.

It was agreed that this document must form the basis of future progress. It is important to establish, even at at this early stage, material support from the Ministry of Health. Support has been agreed, in principle, by the Ministry and the World Health Organization.

A proposal made to Prof. Orinda by Mr Russell on behalf of Randox Laboratories Ltd would enable a pilot programme for 13 laboratories to be established for one 6-month cycle of the Randox International Quality Assessment Scheme. The estimated cost of this would be approximately USD 5000, and it was strongly recommended that this offer should be accepted, thereby enabling the establishment of a quality assessment programme. It would also allow a review of the performance, both absolute and relative, of a significant group of laboratories over a sustained period of time. Additionally, it would give an impetus to maintain and expand such a programme through the steering group envisaged in the recommendations, and add impetus to the establishment of an internal quality control programme in those laboratories that do not have one at the present time.

Looking to the future, the steering group may find it helpful to have outside experts visit Kenya, to comment and advise on how laboratories perform and how their performance might be improved. If this principle is agreed to, the steering group needs to consider as a matter of some urgency how this might be funded, possibly through an outside international agency, such as UNESCO, which is currently supporting this programme.

Trapping single atoms and ions

Metrology, the science of measurement standards, has recently made use of new precision methods for determining more accurate atomic masses. This advance has been made possible through the study of single ions trapped in electromagnetic fields. The device at the centre of these new developments is a Penning trap, so named for F.M. Penning and used first to confine a single electron. The trap employs a uniform magnetic field to direct an ion into a circular path perpendicular to the field lines. However, this is of itself not enough to trap the ion; as the ion has motion parallel to the field lines - it could, for example, spiral out of the trap in a helical movement. To prevent this form of motion and the lose of the ion a set of three electrodes create an electric field to confine the ion within the ends of the trap, see Fig. 1. Once the ion is caught, its mass may be determined by observing the orbits executed by the charged species in the applied magnetic field—a charged particle in a magnetic field will follow orbits with different periods based on their mass-to-charge ratio. The measurement is made by applying a radiofrequency field which matches the ion's cyclotron frequency, that is, the rate at which it completes a circular orbit due to the applied magnetic field. The cyclotron frequency is a direct measure of the mass-to-charge ratio.

Recent advances have followed from: the development of much more stable and uniform magnetic fields, a detailed knowledge of the extent of the trapping electric field, and the ability to isolate and examine only one ion, which may be singly or multiply charged, in any trap. Indeed, measuring a single multiply charged ion provides a higher signal-to noise ratio, as the optimum signal-to noise ratio for a charged species in a Penning trap is proportional to the total charge present on the trapped species. In addition, use of multiply charged ions allows systematic checks through the comparison of results from different charge states of the same element. By comparing the cyclotron frequencies of a sample ion and a carbon ion, alternately trapped in the same environment, it is now possible to measure atomic mass ratios with an precision that is more than 10 times better than any previous technique.

The full name for this device is a Penning Trap Mass Spectrometer (PTMS). The European version of this device differs slightly from those found in the US. In Europe, the ion is excited by the radiofrequency field, then is ejected from the trap along the direction of the magnetic field and drifts towards a particle counter situated at the centre of the field region. When the applied driving frequency matches the cyclotron frequency, the ion's time of flight towards the counter reaches a minimum. This scheme is particularly useful for unstable isotopes with short lifetimes. Such a device has been used in conjunction with a beam of multicharged ions from the Stockholm CRYSIS accelerator to measure

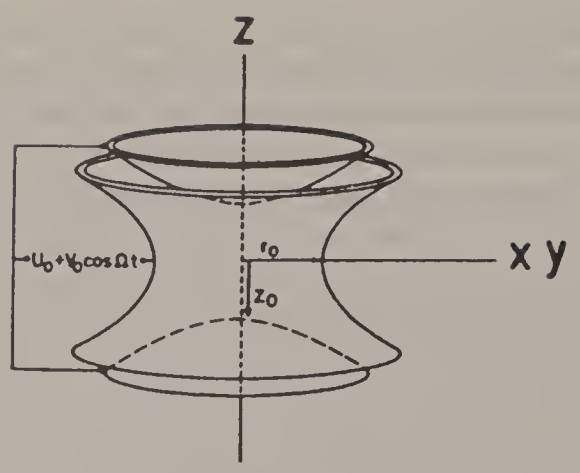

Fig. 1 Schematic of a radiofrequency quadrupole trap for ions. The electrodes are shown as is the direction of the constraining oscillating ($V(t) = u_0 + V_0\cos\omega t$) field.

the atomic mass of ^{28}Si.

By contrast, the United States' version of a PTMS makes a measurement while the ion is circulating within the trap. When the ion is near an electrode surface, it induces a small electric current within the electrode. By probing this small induced circulating current it is possible to determine the cyclotron frequency. This instrument, allows one to capitalise on the inherent stability of the confinement trap—an ion may be confined for several days.

The PTMS at Washington State University has, for example, been used to measure the mass difference between tritium, ^3_1H, and ^3_2He to one part in 10^9—relative to the average ion mass. The tritium atom consisting of one electron, one proton and two neutrons; while the helium atom is made up of two electrons, two protons and one neutron. This mass difference has considerable significance for the possible nonzero rest mass of the neutrino. This PTMS has also recently improved the value of the proton to electron mass ratio. Equally impressive, have been the results from the PTMS at MIT which has, amongst other things, improved the accuracy of the mass of the neutron by a factor of 6. For example, accurate measurements of the relative masses of $\{^{14}_7N—^{14}_7N\}^+$ and $\{^{13}_6C—^{16}_8O\}^+$, that is, cations of particular isotopes of molecular nitrogen and carbon monoxide are different by the mass of a neutron. Both molecular ions cations contain 13 electrons and 14 protons, but the nitrogen cation has 14 neutrons and the carbon monoxide cation contains 15 neutrons.

With such ever increasing precision, it is expected that still greater improvements in various fundamental constants will soon become possible. The MIT group believe that the inherent accuracy of such a device is a part in 10^{10}.

The electromagnetic fields necessary to trap ions can also be provided by light beams. A propagating light beam has associated oscillating electric and magnetic fields. The electric field of a light beam is proportional to the square root of its intensity, and the associated oscillating magnetic field is a factor of $1/c$ (c being the speed of light) of the electric field.

The use of lasers to trap atomic species is a booming business. For example, neutral atoms may be manipulated with the force exerted upon them by laser photons. With powerful lasers this force may be large, the atoms are cold with almost no forward momentum to overcome, and it may be delicately adjusted. Consider a powerful focused laser beam resonant with an absorption in, for example, a lithium atom; the electric field, E, associated with the light beam can be of order 10^7 V/m, this beam after focusing would have a diffraction limited waist of 10^{-6} m yielding an electric field gradient associated with the light beam of 10^{13} V/m^2. This inhomogeneous electric field, ∇E, will exert a force, F, on a lithium atom through the electric dipole moment, μ, induced in the atom by the electric field of the light beam interacting with the atomic polarizability of the lithium atom, α ($\mu \approx \alpha E$). That is, $F \approx \nabla E \cdot \mu \approx \alpha \nabla E \cdot E$. For a resonant polarizability we may readily take $\alpha \approx 10^{-38}$ $C^2m^2J^{-1}$, yielding for the force exerted by a laser beam on a lithium atom at resonance, $F \approx 10^{-18}$ Newtons (m kg s^{-2}). This force acting over the beam waist yields an interaction potential, of order, 10^{-24} J, which is larger than kT for these cooled atoms. Consequently, the applied optical force will accelerate the neutral atoms.

This type of atom trap is termed a magneto-optical trap (MOT). Very cold atoms (that is, no velocity) at temperatures well below a thousandth of a degree absolute above absolute zero, are trapped at the zero point in the centre of a weak magnetic field, intersected by three counterpropogating pairs of perpendicularly directed laser beams.

Groups at the State University of New York, Stony Brook, and the Lawrence Berkeley Laboratory have recently been particularly active in this field. The Stony Brook team produced ^{79}Rb (half-life 22.8 min) and neutralized them in a yttrium tube. Some of the atoms fell into the MOT at the centre of the apparatus. Once trapped, the individual radioactive atoms were available for a variety of spectroscopic experiments.

The Lawrence Berkeley group have trapped ^{21}Na, and are interested in observing the β decay from trapped individual atomic nuclei of ^{21}Na to investigate aspects of the weak force. In β decay, a decomposing unstable (radioactive) nucleus emits an electron or positron together with a neutrino or antineutrino. The electron (positron) and neutrino (antineutrino) that emerge from the decaying nuclei prefer to spin in the same direction with respect to their directions of motion. The mirror image of this process is suppressed. For this reason, β decay is said to violate the fundamental symmetry known as parity. A very precise observation/measurement of the β decay of ^{21}Na will yield new information about parity invariance in the weak force, the force responsible for radioactive decay.

Both of the above groups are attempting to trap isotopes of the heaviest alkali ion, francium. Here the interest is in observing the coupling of the weak and electromagnetic forces, which increases rapidly with nuclear charge.

Calculations related to the above experiments have recently been made on the trapping of molecules by two Harvard chemists, Bretislav Friedrich and Dudley Herschbach (*Phys. Rev. Lett.* 1995, **74,** 4623–4626). For cooling and trapping molecules, the situation is much more complex than for atoms. Whereas a molecular ion may undergo spontaneous dissociation before, or while, being trapped, the presence of vibrational and rotational degrees of freedom complicates the routes for energy transfer within excited molecular species.

If the molecules carry a permanent molecular electric dipole moment, then applied laboratory electromagnetic fields may be used to slow and trap a dipolar molecule—an applied field-gradient will exert a torque on an electric dipole moment. Bretislav & Herschbach have recently shown, however, that it is in general possible to cool and trap any polarizable molecule, provided the parallel and perpendicular components of the, second rank, molecular polarizability (the molecular property which gives rise to Rayleigh and Raman scattering) are sufficiently different. That is, the molecule is anisotropically polarizable, as in CO_2 or C_6H_6.

Bretislav & Herschbach have considered the behaviour of anisotropically polarizable molecules in the electric field associated with a powerful infrared laser. Their calculations are similar to those outlined above, except that the incident laser radiation is not resonant with an atomic absorption line of a visible laser, but with an allowed infrared absorption of a small polyatomic, a molecular vibration in the frequency region of a few thousand wavenumbers. However, there will still be a significant resonant enhancement of the molecular polarizability.

The force exerted, at resonance, by the infrared radiation on the absorbing molecule is not great, however, if the molecule is conventionally cooled sufficiently then the weak orienting force of the infrared radiation may be observed. Experiments at Saclay, Paris, have demonstrated the alignment of CO molecules with a CO laser. However, liquid ^{3}He was first used to cool the, initially hot, CO molecules (*J. Phys.* 1992, **B25**, L497).

Bretislav & Herschbach consider the trapping of molecules as diverse as CO_2 and C_{60}. They estimate that with current laser technology, and for the most suitable cooling conditions, it would be possible to achieve trapped concentration of over 10^8 molecules cm^{-3}. From previous experience, such experiments if undertaken would yield results which would certainly influence our understanding of molecular structure.

Manipulating atoms and molecules individually is, however, more than a mere sport, but it is increasingly able to yield new insights into the interaction of matter with radiation. A group at the *Laboratoire Kastler Brossel*, Paris (A. Steane *et al. Phys. Rev. Lett.* 1995, **74**, 4972–4975), have managed to modulate the phase of the de Broglie waves that represent the physical motion of atoms in circumstances where the rules of quantum mechanics apply. This is more than gimmickry, in that quantum mechanics is one of the most successful of all theories used in the physical sciences, and to find new links between it and those areas of science considered 'classical', such as the kinetic motion of heavy atoms, is always important.

Caesium atoms are 'dropped' onto a virtual mirror from a magneto-optical trap. The atoms are initially cooled in two magneto-optical traps. In the first trap, Cs atoms are cooled to 5°K by detunning the lasers, which define the trap, by about 9 linewidths of the atomic resonance. This creates an 'optical molasses' within which the atoms move as if confined to a viscous fluid. Then the lasers are detunned further, thus reducing the interaction between the atoms and the light field to such an extent that the atoms fall out of the trap. Indeed, the Cs atoms fall about 70 cm into a second trap which operates in a better vacuum than the first, thereby extending the time for which an atom may be trapped. It is from this trap, containing much cooler atoms, that the atoms fall onto the light mirror.

This virtual, or light, mirror is infact a pattern of oscillating electric field generated by an intense laser beam. The force between the atom and the mirror comes from the gradient of the electric field of the light beam acting on the large atomic polarizability (see above). This virtual or optical mirror is modulated between reflectivity and transparency, with the result that the Cs atoms which are reflected have their kinetic energy modulated. This modulation of the kinetic energy of the atom is equivalent to the modulation frequency of the virtual mirror. This is demonstrated by allowing the atoms to bounce up to the top of their ballistic trajectory before measuring the position at which they come down again. The bouncing of the heavy Cs atoms was timed, and the time required for a Cs atom to move vertically upwards and then down again is a measure of its initial velocity, which must be $2gt$, where g is the acceleration due to gravity at Paris and t the time. These initial experiments suggest that a much more precise method for the measurement of g.

In what is undoubtedly be one of the most important experiments undertaken todate with lasers, M. H. Anderson, J.P. Ensher, M.R. Matthews, C.E. Wieman and E.A. Cornell of the University of Colorado, USA (*Science* 1995, **269**, 198–201), have succeeded in observing a Bose–Einstein condensation in a dilute vapour of rubidium-87 atoms—thereby creating a new

state of matter.

The observation of a Bose–Einstein condensation, predicted by S.N. Bose and Einstein in 1924–1925, builds on many of the technical advances discussed above—the laser cooling of atoms. However, Anderson *et al.* have taken the cooling to a much greater level, and cooled a few thousand atoms of rubidium to 20×10^{-9} °K. At such a low temperature, and at an appropriate number density, the atoms spontaneously condense into a new material. This new material is not like conventional solid rubidium, but each atom in the new low temperature condensate senses the presence of every other atom in the condensate. Each atom in the condensate is characterised by a de Broglie wavelength, the phases of whose wavefunctions are the same for all the atoms. That is, the atoms have lost sufficient energy to fall into a single quantum state. This collective occupation of the same quantum state is possible for Bose particles, or Bosons (particles whose angular momentum is an integer multiple of $h/2\pi$). Unlike electrons, any number of rubidium-87 atoms can occupy a single quantum state, however, only one electron can occupy each quantum state of an atom; electrons are Fermi–Dirac particles, or Fermions (particles whose angular momentum is a half integer multiple of $h/2\pi$).

As all the condensed atoms are in the same quantum state, they have the same wavefunction which means the condensate is coherent—just like the photons produced in a laser and the condensate may be thought of as a single 'super atom'. Another example of coherence in a solid is a material which is a superconductor. In a superconductor, all the electrons are in the same quantum state, however, these coherent electrons are present in a solid to which they are strongly coupled, and it is this coupling which has made an understanding of the new cuprate superconductors so elusive. However, in the new rubidium Bose–Einstein condensate the atoms are coherent and there is no surrounding perturbing matrix, consequently, it is likely that the study of Bose–Einstein condensates will lead to advances in many fields of chemistry and physics.

News

IUPAC Affiliate Membership Database

Due to restructuring and reorganization at the Oxford Secretariat, it has been decided to discontinue the IUPAC Affiliate Membership Database. Consequently, IUPAC Affiliate Membership Registration Forms will no longer be dispatched, and the Affiliate documents included with this issue of Chemistry International refer only to Affiliate membership.

1995 Nobel Prizes

The 1995 Nobel Prize for Chemistry has been awarded to three scientists for their investigation of the chemistry that affects the amount of ozone in the stratosphere.

F. Sherwood Rowland, Professor of Chemistry at the University of California, Irvine; Mario Molina, Professor of Chemistry in the Departments of Chemistry and of Earth, Atmospheric and Planetary sciences at the Massachusetts Institute of Technology; and Paul Crutzen, Director of the Department of Atmospheric Chemistry of the Max Planck Institute for Chemistry, Mainz, Germany, have shared this year's prize in chemistry.

Twenty-five years ago, Crutzen showed that naturally occurring nitrogen oxides catalyticaly destroy ozone, thereby helping to regulate its concentration in the stratosphere. Ozone is continually created and consumed in the stratosphere by the action of intense ultraviolet solar radiation on molecular oxygen. Molecular oxygen absorbs strongly in the ultraviolet and this absorption can lead to dissociation. The liberated oxygen atoms can then react with other oxygen molecules to produce ozone. However, ozone also absorbs strongly in the ultraviolet to a dissociative state. Consequently, ozone is formed and consumed under the influence of hard solar radiation. Crutzen was the first to point out that nitrogen oxides (other open shell species with complex absorption spectra in the visible and ultraviolet) could also participate in the decomposition pathways of stratospheric ozone:

$$O_3 + h\nu \rightarrow O_2 + O$$

$$NO + O_3 \rightarrow NO_2 + O_2$$

$$NO_2 + O \rightarrow NO + O_2$$

Net: $2O_3 \rightarrow 3O_2$

Crutzen also pointed out that the closed shell, relatively unreactive, molecule nitrous oxide, N_2O, which is naturally liberated from soil, can rise into the atmosphere and be decomposed by hard solar radiation in the stratosphere. In this way, a fraction of the N_2O is converted into the more reactive nitrogen oxide radicals which may then participate in the destruction of stratospheric ozone.

In 1974, Rowland and Morina recognized that chlorine atoms liberated photochemically from available

chlorofluorocarbons (CFCs) could also react with ozone. Indeed, more than a decade before the discovery of the ozone hole above the Antarctic these chemists warned that continued emissions of CFCs could deplete the atmospheric ozone layer and thereby expose the earth's surface to increasing amounts of harmful hard ultraviolet solar radiation.

The CFCs, used as refrigerants, foam blowing agents, industrial solvents, etc., are inert and so survive until they move upwards into that part of the stratosphere where they are photochemically decomposed by hard solar radiation. Thereby liberating chlorine atoms that attack the ozone to be found in that level of the atmosphere:

$$O_3 + h\nu \rightarrow O_2 + O$$

$$Cl + O_3 \rightarrow O_2 + ClO$$

$$ClO + O \rightarrow Cl + O_2$$

Net: $2O_3 \rightarrow 3O_2$

'By explaining the chemical mechanism that affect the thickness of the ozone layer, the three researchers have contributed to our salvation from a global environmental problem that could have catastrophic consequences,' says the Royal Swedish Academy of Sciences, which awards the Nobel prize (*C&E News*, 16 October 1995).

Having explained a potential catastrophe, these authors, however, had great difficulty in getting their ideas accepted. Rowland and Molina spent years defending their ideas from critics reluctant to accept its implications for the useful, cheap, and ubiquitous CFCs. In the United States, their warning lead to a ban on the use of CFCs in aerosols. Elsewhere, however, little concern was expressed until a team of scientists from the British Antarctic Survey reported in 1985 that severe ozone depletion was occurring over Halley Bay in Antarctica.

This observation was a surprise, because Rowland and Molina had estimated that ozone depletion by chemical loss should be greatest at the level of the tropics where solar radiation was most intense. Unravelling the reasons for the large polar ozone loss has involved international collaboration to which all three participants have contributed. By 1990 it was clear that the low temperatures above the southern continent are critical, and that ozone depletion here is not a result of homogeneous gas phase reactions, but involves heterogeneous reactions taking place on the surface of ice particles in polar stratospheric clouds. These reactions, in the dark of the polar winter, prime the cloud particles for photochemical ozone destruction when the sunlight returns in the spring.

This work led to an explosion of interest in atmospheric chemistry, and has led, in conjunction with the discovery of the ozone hole, to the phasing out of CFCs under the Montreal Protocol on *Substances That Deplete the Ozone Layer*.

However, the science behind an explanation of the ozone hole is currently under attack as the 1996 deadline for the abolition of the use of CFCs approaches. For example, last month a Subcommittee of the US Congress held a meeting entitled Stratospheric Ozone: Myths and Realities (*C&E News*, 9 October 1995). Legislation has been put before Congress that would weaken US policies to protect the ozone layer. Indeed, some of those who do not support the idea of the anthropomorphic origin of the ozone hole term the idea as the *fin de siècle* madness of the 20th century.

'I would hope that this award would give pause to people who have been arguing ozone depletion is just political rhetoric', says Robert T. Watson, Associate Director for the Environment at the White House Office of Science and Technology Policy. 'Nobel prizes are not given out lightly; they are given after careful consideration that the work will stand the test of time. This prize gives recognition to environmental issues as part of credible mainstream science.' (*C&E News*, 16 October 1995).

This year's Nobel Prize for Physics was shared by Martin L. Perl of Stanford University, California, for his discovery of the tau lepton in the early 1970s, and Frederick Reines, of the University of California at Irvine, for the detection of the neutrino almost 20 years earlier.

Both of these discoveries, although widely separated, significantly advanced our understanding of the subatomic world and helped to create the so-called Standard Model of particle physics, in which six leptons—consisting of the electron, the muon, the tau and three corresponding neutrinos, in addition to six associated quarks, are the elementary constituents of matter.

The existence of the neutrino was postulated by Pauli in 1933. During the process of beta decay an atomic nucleus emits an electron or positron, and simultaneously changes into the nucleus of a different element. Early experiments showed that energy was irretrievably lost in the process, suggesting that the principle of energy conservation might have to be abandoned at subatomic dimensions. To avoid this drastic conclusion, Pauli proposed that energy was carried away by an uncharged and massless fundamental particle. This was a radical suggestion at the time as only three fundamental subatomic particles were then known—the electron, proton and neutron. Two decades later, Reines and his collaborator announced the discovery of the neutrino, calling it 'the smallest bit of material reality ever conceived by man.'

The discovery of the tau was made possible by the construction, at the Stanford Linear Accelerator Center, of a new accelerator (SPEAR) which Perl began to use

in 1973. In his experiments, electrons and positrons were collided at high energies, producing a large number of secondary particles.

Within a proton or a neutron there are three component quarks which move under the influence of messenger particles called 'gluons'. When protons and neutrons are assembled into a nucleus, the inter-quark attraction carried by the gluons dominates the electric repulsion between protons. However, there is a third force at work within the nucleus. A neutron occasionally decays radioactively, becoming a proton and releasing an electron and a neutrino. Here, the weak nuclear force, which is less than 10^6th of the strength of the strong nuclear force, and carried by the W and Z particles (each about a 100-fold heavier than the proton) dominates the subatomic range. The contrast between the strong and the weak nuclear forces gives rise to two distinguishable classes of particles—leptons and hadrons. Leptons, such as the electron and the neutrino do not feel the strong force and are so small that their dimensions are not determinable—if they have any dimensions at all. Hadrons, such as the proton and the neutron, feel all forces and have a measurable size. There are hundreds of hadrons, but because they contain smaller particles (quarks) they can be grouped into related families; containing three quarks (e.g. protons or neutrons) or a quark and an antiquark (e.g. pions). Despite their very different properties, quarks and leptons can themselves be related. Most of the world which is familiar to us can be explained in terms of a quartet of particles containing two kinds of quark ('up' and 'down'), together with the electron and its associated neutrino.

Chemistry for Life

Celebration of 75 years of IUPAC

On 26 June 1994, IUPAC's 75 years were celebrated by the National Committee for Chemistry (NCC) in Belgium (National Adhering Organization to IUPAC) by inviting over 600 chemistry teachers, from all over Belgium, to a symposium. Prof. P. De Bièvre, President of NCC, highlighted the important role chemistry teachers have in determining the image of chemistry in the minds of young adults who are about to choose their field of study. Prof. De Bièvre pointed to the extraordinary variety of 'chemicals' which daily enhance the quality of life: pharmaceuticals, materials, food, and agents against infection. Both the Flemish and Walloon ministers of education brought an official message of appreciation and encouragement for the chemistry teachers.

Belgian chemistry teachers at the symposium to celebrate 75 years of IUPAC.

The President of the Federation of Belgian Industries stressed the importance of chemistry for employment, quoting the large numbers of employees in the Belgian chemical industry. Prof. Dr P. Janssen, founder and research director of Janssen Pharmaceuticals, explained the key importance, but also the complexity of, the fight against AIDS, outlining the approaches of pharmaceutical research to this field.

Nobel laureate Chr. de Duve from the University of Louvain-la-Neuve gave an extraordinarily clever overview of what had happened—and continues to happen—in matters of chemistry at, and since, the Big Bang. The emerging image of the universe is one where life abounds in a multitude and complexity which can only leave us staggered with amazement and admiration.

During the ensuing reception, the AGFA-GEVAERT chemical company (Antwerp) distributed to each teacher a 3 kg package of teaching aids for chemistry consisting of colour transparencies with associated texts, DIDAC-1 (for an example of these aids see Fig. 1). These transparencies were specially prepared to render chemistry teaching easier for the teacher and more attractive to the student. The teachers were also able to meet the speakers during the reception.

Paul De Bièvre
(President, National Committee on Pure and Applied Chemistry of Belgium)

Members of the Belgian National Committee for Chemistry.

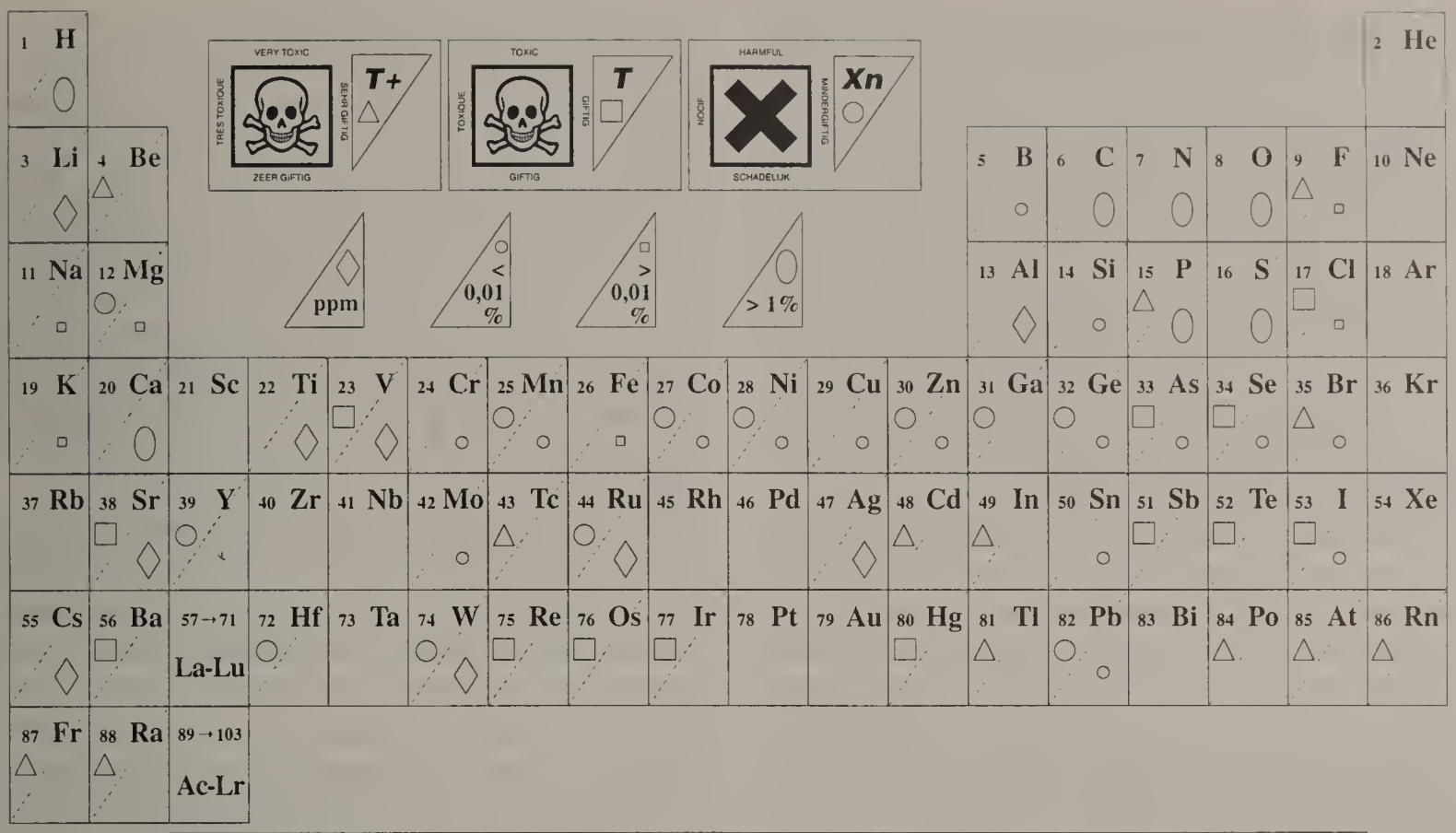

Fig. 1 Part of the DIDAC-1 set of teaching aides, showing the toxicity of various chemical elements and demonstrating solution equilibria.

Change of Name for Swiss Chemical Societies

The duties and member societies of the Swiss Committee of Chemistry have gradually been taken over by the New Swiss Chemical Society (NSCS). Consequently, it has been decided to officially close the Swiss Committee of Chemistry as of 31 December 1995. From this date, the National Adhering Organization will be the New Swiss Chemical Society.

The address of the society is:

Neue Schweizerische Chemische Gesellschaft,
c/o Ciba, K–25.5.02
4002 Basel, Switzerland
Tel.: +41 61 696 66 26
Fax: +41 61 696 69 85.

Antimatter

Antimatter, so beloved of science fiction writers as the perfect power source, has come of age. In an experiment at the *Conseil Européen pour la Recherche Nucléaire* (CERN), otherwise known as the European Laboratory for Particle Physics, near Geneva, scientists have succeeded in creating 11 atoms of antihydrogen.

The years which immediately followed the first Solvay conference in October 1927 have been called the golden age of atomic physics. Quantum mechanics was just over two years old, but much had already been done to establish a formal structure for the new theory. The conceptual basis for this new theory had been clarified with the introduction of the uncertainty principle and complementarity. Quantum mechanics and quantum statistics had come together and allowed the world of macroscopic thermodynamics to be related to the world of subatomic particles. There was, however, no marriage of quantum mechanics and relativity.

It was Paul Dirac who in 1928 first developed a theory of the electron in an electromagnetic field which satisfied the relativistic requirement of invariance (unchanging) under a Lorentz transformation—a transformation from one set of space–time coordinates to another set of such coordinates moving with constant velocity to the first set of coordinates. On attempting to factorise his relativistic Hamiltonian, Dirac discovered that electron spin arose as a natural consequence of the relativistic correction, when compared to a non-relativistic Hamiltonian. Unfortunately, his relativistic wave equation gave twice as many energy levels as were called for, and as were obtained from solution of the non-relativistic wave equation. Dirac showed how this apparent flaw arose from the necessity of having to consider the

two roots of the energy–momentum–mass relation ($E^2 = c^2p^2 + m^2c^4$), where c is the velocity of light, m the electron mass and p the electron momentum.

What does one do with the negative energy solutions, 'holes in the vacuum', as Dirac imagined them? Dirac said in 1977, 'I was reconciled to the fact that the negative energy states could not be excluded from the mathematical theory, and so I thought, let us try and find a physical explanation for them.' (*Inward Bound: Of Matter and Forces in the Physical World,* by Abraham Pais. OUP, 1986). Dirac's theory had predicted a particle that was identical to the electron in every way, except that it was positively charged.

These negative energy solutions caused consternation amongst the supporters of non-relativistic quantum mechanics. In 1928, Heisenberg wrote to Pauli saying, 'The saddest chapter of modern physics is and remains the Dirac theory.' In 1931, having taken note of all the numerous objections to his relativistic quantum theory, Dirac said that 'a hole, if there were one, would be a new kind of particle, unknown in experimental physics, having the same mass and opposite charge of the electron.' However, it was in September 1932 that Carl Anderson observed the deflection of particles in a magnetic field which were of opposite character from the deflection of an electron—the first observation of Dirac's antiparticle. The name positron was first used in 1933.

Dirac was a theoretician of the highest order, however, he was a taciturn man not given to understatement. In the preface of his text, *Quantum Mechanics*, he says that his relativistic wave equation (if it could be solved) would explain much of physics and all of chemistry. However, the story of the discovery of antimatter is the story of theory and experiment. The experimentalist, Anderson, who observed the positron five years after its prediction said much later, 'Yes, I knew about the Dirac theory...but I was not familiar in detail with Dirac's work. I was too busy operating this piece of equipment to have much time to read his papers...[Their] highly esoteric character was apparently not in tune with most of the scientific thinking of the day...The discovery of the positron was wholly accidental.' (*Inward Bound: Of Matter and Forces in the Physical World*, by Abraham Pais. OUP 1986).

Whether accidental or not, this combination of theory and experiment lead to one of the triumphs of 20th century physics and showed the way forward in particle physics, indeed, any large scientific problem, with a combination of theory and experiment.

The positrons observed by Anderson were formed by cosmic rays interacting with atoms in cloud chambers. The recent experiments at CERN have set out with the intention of combining such exotic states of matter into larger atomic (antiatomic) building blocks. The physicists at CERN started with a beam of antiprotons—a proton with a negative charge—and allowed it to interact with a beam of xenon atoms. Antiprotons have been known for some time, as they are produced by colliding protons at very high energies. Because of the low number density of antiprotons in a particle beam, there are only a few collisions between the antiprotons and the nuclei of the xenon atoms which lead to the expulsion of an electron and a positron from the xenon nuclei. In even rarer instances in the interacting beams, the positron liberated from the xenon nuclei will be able to combine with the antiprotons present to produce an atom of antihydrogen. That is, a hydrogen atom composed of an antiproton and a positron.

The Low Energy Antiproton Ring (LEAR) at CERN where these experiments were carried out is so shaped that four straight sections are joined by curved pieces which contain powerful electromagnets which bend charged particles around the curvature, thus allowing them to complete a circuit of the apparatus. The researchers created antihydrogen in one of the straight sections, and were able to detect it because it would not be deflected by the corner deflecting magnetic field and so would collide with the apparatus wall. In actuality, a detector is placed at the point where the antihydrogen would collide with the wall, and here the antihydogen was stripped down into its component parts—an antiproton and a positron. Each liberated positron annihilated with an electron in the detector to produce a gamma ray which was readily monitored.

Protons (p) hit a beryllium target at 27 GeV and scatter from the atomic nuclei giving protons and antiprotons ($\bar{p}$).

$$p + p \rightarrow p + \bar{p}$$

The antiprotons ($\bar{p}$) interact via a two-photon process with a xenon nuclei (Z) creating an electron/positron pair (e^-e^+), the positron (e^+) of this pair may then be captured by the antiproton giving an atom of antihydrogen ($\bar{H}$). The probability of all these processes is of the order of 10^{-17} per second.

$$\bar{p} + Z \rightarrow \bar{p} + e^-e^+ + Z \rightarrow \bar{H} + e^- + Z$$

For the future, one of the goals of such experiments is to produce a sufficient concentration of antihydrogen to perform high-resolution laser spectroscopic measurements. At very high frequency resolution, one may determine the hyperfine coupling constants which show the coupling between the electron and nuclear dynamics within the atom. Such measurements are well established in ordinary hydrogen, and have led to detailed measurements of the Rydberg constant. However, such measurements in antihydrogen, with its differently charged components, would be a significant test of the relativistic wave equation.

Names and Addresses

Full details (names, addresses, telephone/telex/Fax numbers and E-mail) of the officers of IUPAC bodies were published in *Chemistry International* 1995; **17**(6): 215–226. The IUPAC Secretariat has been notified of the following changes:

Prof. Enrico Baciocchi (Secretary, Commission III.2), E-mail: baciocchi@axcasp.caspur.it

Prof. Donald W. Moss (President, Division of Chemistry and Human Health), 42 Greenways, Esher, Surrey KT10 0QD, UK. Tel.:/Fax: +44 181 398 5143.

Dr Thomas J. Perun (Chairman, Commission on New Technologies and Special Topics, VII.M.3), Abbott Laboratories, Department 467, Building R-8, North Chicago, Il 60064 4000, USA. Tel.: +1 847 937 8622; Fax: +1 847 938 2258.

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Prof. Gianfranco Scorrano (President, Division III), E-mail: scorrano@pdchor.unipd.it

Dr Yehuda Shevah (Chairman, Commission VI.3), Tel.: +972 3 692 4279; Fax: +972 3 692 4280.

Dr T. Vo-Dinh (Chairman, Commission V.4), Tel.: +1 423 574 6249; Fax: +1 423 576 7651; E-mail: tvo@ornl.gov

Recent Reports

In this section we publish summaries of the most recent IUPAC recommendations on nomenclature and symbols and technical reports. The full texts of these recommendations and reports are published in *Pure and Applied Chemistry*

Nomenclature in evaluation of analytical methods, including detection and quantification capabilities (IUPAC Recommendations 1995)

Synopsis: This IUPAC nomenclature document has been prepared to help establish a uniform and meaningful approach to terminology, notation and formulation for performance characteristics of the Chemical Measurement Process (CMP). Following the definition of the CMP and its Performance Characteristics, the document addresses fundamental quantities related to the observed response and calibration, and the complement to the calibration function: the evaluation function. Performance characteristics related to precision and accuracy comprise the heart of the document. These include measures for the means or 'expected values' of the relevant chemical quantities, as well as dispersion measures such as variance and standard error. Attention is also given to important issues involving: assumptions, internal and external quality control, estimation, error propagation and uncertainty components, and bounds for systematic error. Special treatment is given to terminology and concepts underlying detection and quantification capabilities in chemical metrology, and the significance of the blank. The document concludes with a note on the important distinction between the Sampled Population and the Target Population, particularly in relation to the interlaboratory environment.

This Report was prepared for publication by Lloyd A. Currie (Chemical Science and Technology Laboratory National Institute of Standards and Technology, Gaithersburg, MD 20899, USA) for the Commission on Analytical Nomenclature of the Analytical Division. The full details are to be found in Pure Appl. Chem. *1995, **67**, 1699–1723.*

Nomenclature, symbols, units and their usage in spectrochemical analysis—IX. Instrumentation for the spectral dispersion and isolation of optical radiation (IUPAC Recommendations 1995)

Synopsis: This document deals with nomenclature, symbols and their usage in the field of instrumentation for the dispersion and isolation of optical spectra in the wavelength region from 50 nm to 1 mm, as applied in analytical atomic and molecular emission, absorption and fluorescence spectroscopy. The whole subject is divided into 10 chapters dealing with various aspects of dispersive and non-dispersive spectral apparatus including spectral filters and interferometers. Definitions are given for spectral instruments with and without detection and measuring facilities. The properties of optical components of dispersive and non-dispersive spectral instruments are defined in detail, with emphasis on such fundamental figures of merit as spectral purity, resolution, resolving power, conductance of optical systems, characteristic wavelengths and polarization. Terms closely related to the optimum use of spectral instruments, e.g. optimal slit width and height, theoretical and practical effective spectral linewidth and line-to-background radiant power ratio are given. Terms for

various forms of mountings for spectral apparatus are included in the vocabulary.

This Report was prepared for publication by L. R. P. Butler[1] and K. Laqua[2] ([1]Spectro Analytical Instruments, PO Box 17063, Groenkloof 0227, RSA; [2]Grüner Weg 2, D-44267 Dortmund, Germany) for the Commission on Spectrochemical and other Optical Procedures of Analysis of the Analytical Division. Full details are to be found in Pure Appl. Chem. *1995, **67**, 1725–1744.*

Nomenclature, symbols, units and their usage in spectrochemical analysis—XI. Detection of radiation (IUPAC Recommendations 1995)

Synopsis: This report is the 11th in the series on Spectrochemical Methods of Analysis issued by IUPAC Commission V.4. It is concerned with Radiation Detection as used in analytical atomic and molecular emission, absorption, and fluorescence spectroscopy in the X-ray and optical wavelength region (i.e. from 10 pm to 1 mm). The present report has five main sections: terms relating to (a) fundamental properties of detectors, (b) thermal detectors, (c) photo-emissive detectors (d), semiconductor detectors, and (e) spatially resolving detectors. Although still of considerable importance, photographic emulsions are not included.

This Report was prepared for publication by K. Laqua[1], B. Schrader[2], G. G. Hoffmann[2], D. S. Moore[3] and T. Vo-Dinh[4] ([1]Gruner Weg 2, D-44267 Dortmund, Germany; [2]Institut fur Physikalische und Theoretische Chemie, Universitat-GH-Essen, D-45117 Essen, Germany; [3]Chemical Science and Technology Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA; [4]Advanced Monitoring Development Group, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6101, USA) for Commission on Spectrochemical and other Optical Procedures of Analysis of the Analytical Division. The full details are to be found in Pure Appl. Chem. *1995, **67**, 1745–1760.*

Nomenclature, Symbols, Units and their Usage in Spectrochemical Analysis: Cumulative Index of Terms: Parts I—XIII

A series of documents dealing with nomenclature, symbols and units used in spectrochemical analysis has been issued by IUPAC to date in 13 parts:

Part I. General Atomic Emission Spectroscopy [*Pure Appl. Chem.* 1972, **30**, 653–679].

Part II. Data Interpretation [*Pure Appl. Chem.* 1976, **45**, 99–103].

Part III. Analytical Flame Spectroscopy and Associated Non-Flame Procedures [*Pure Appl. Chem.* 1976, **45**, 105–123].

Part IV. X-ray Emission Spectroscopy [*Pure Appl. Chem.* 1980, **52**, 2541–2552].

Part V. Radiation Sources [*Pure Appl. Chem.* 1985, **57**, 1453–1490].

Part VI. Molecular Luminescence Spectroscopy [Pure Appl Chem. 1984, **56**, 231–345].

Part VII. Molecular Absorption Spectroscopy, Ultraviolet and Visible (UV/VIS) [*Pure Appl. Chem.* 1988, **60**, 1449–1460].

Part VIII. Nomenclature System for X-ray Spectroscopy [*Pure Appl. Chem.* 1991, **63**, 735–746].

Part IX. Instrumentation for the Spectral Dispersion and Isolation of Optical Radiation [*Pure Appl. Chem.* 1995, **67**, 1725–1744].

Part X. Preparation of Materials for Analytical Atomic Spectroscopy and other Related Techniques [*Pure Appl. Chem.* 1988, **60**, 1461–1472].

Part XI. Radiation Detectors [*Pure Appl. Chem.* 1995, **67**, 1745–1760].

Part XII. Terms Related to Electrothermal Atomization [*Pure Appl. Chem.* 1992, **64**, 253–259].

Part XIII. Terms Related to Chemical Vapour Generation [*Pure Appl. Chem.* 1992, **64**, 261–264].

This Report was prepared for publication by D.S. Moore[1], T.A.M. Ure[2] and L.R.P. Butler[3] ([1]Chemical Sciences and Technology Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA; [2]Department of Pure and Applied Chemistry, University of Strathclyde, Glasgow GI 1XL, UK; [3]PO Box 17063, Groenkloof 0227, Republic of South Africa) for Commission on Spectrochemical and other Optical Procedures of Analysis of the Analytical Division. The full details are to be found in Pure Appl. Chem. *1995, **67**, 1761–1779.*

Determination of total chlorophyll pigments in crude vegetable oils: Results of a collaborative study and the standardized method (Technical Report)

Synopsis: The development, by collaborative study, of a standardized method for the determination of chlorophyll pigments (mainly pheophytins, which are produced by loss of magnesium from the molecules of respective chlorophylls) in crude vegetable oils is described. The chlorophyll pigments are determined by spectrophotometric measurement at 670 nm.

This Report was prepared for publication by J. Pokorny[1], L. Kalinovai[1] and P. Dysseler[2] ([1]Department of Food Science, Faculty of Food and Biochemical Technology, Prague Institute of

Chemical Technology, Technicka St. 5, CZ-166 28 Prague 6, Czech Republic; [2]Institut Meurice Chimie, Centre d'Enseignement et de Recherches des Industries alimentaires et Chimiques, Avenue Emile Gryzon 1, B-1070, Bruxelles, Belgium) for the Commission on Oils, Fats and Derivatives of the Analytical Division. The full details are to be found in Pure Appl. Chem. *1995, **67**, 1781–1787.*

The electrical conductivity of cubic stabilized zirconia: The results of a IUPAC collaborative study (Technical Report)

Synopsis: The purpose of the present work is to compare data obtained by impedance spectroscopy in several laboratories on the same ionically conductive materials. Yttria-doped zirconia, stabilized under the cubic form, was selected. Measurements were carried out in the temperature range 200–600°C to get the bulk and the grain boundary contributions to the material impedance. The data were analysed centrally. The DC conductivity could be obtained with a fair accuracy. Problems concerning the determination of AC properties are clearly pointed out. Some recommendations are made to improve the general reliability of measurements made with the aid of impedance spectroscopy.

This Report was prepared for publication by P. Abélard and J. F. Baumard (Laboratoire de Matériaux Céramiques et Traitements de Surface, ENSCI, 47 Avenue Albert Thomas, 87065 Limoges Cedex, France) for the Commission on High Temperature and Solid State Chemistry of the Inorganic Chemistry Division. Full details are to be found in Pure Appl. Chem. *1995, **67**, 1891–1904.*

Absolute methods in analytical chemistry (Technical Report)

Synopsis: There is an increasing tendency to obtain the analytical result on the basis of numerical calculations deriving from the theoretical model of the phenomena responsible for formation of an analytical signal. Such procedures, where the calculations are based on universal quantities and fundamental physical constants only, may be termed absolute methods. There are a number of terms which refer to methods which do not need direct experimental calibration which, however, cannot be named absolute. This project indicates also existing examples in various analytical techniques, where the term 'absolute' is more or less justified.

This Report was prepared for publication by A. Hulanicki (Wydziat Chemii, Uniwersytet Warszawski, ul. L. Pasteura 1, PL-02 093 Warszawa, Poland) for the Commission on General Aspects on Analytical Chemistry of the Analytical Chemistry Division. Full details are to be found in Pure Appl. Chem. *1995, **67**, 1905–1911.*

Nomenclature, symbols, units and their usage in spectrochemical analysis—XV. Laser-based molecular spectroscopy for chemical analysis—laser fundamentals (IUPAC Recommendations 1995)

Synopsis: This report is 15th in a series on Spectrochemical Methods of Analysis issued by IUPAC Commission V.4. It is concerned with the fundamental properties of lasers as used in analytical molecular spectroscopy in the optical wavelength region. The present report has five main sections: Introduction to lasers, Types of lasers, Laser propagation, Laser dynamics, and Exploitation of laser properties.

A series of documents dealing with nomenclature, symbols and units used in spectrochemical analysis issued by IUPAC.

Part I [*Pure Appl. Chem.* 1972, **30**, 653–679] is concerned mainly with general recommendations in the field of emission spectrochemical analysis.

Part II [*Pure Appl. Chem.* 1976, **45**, 99–103] gives some basic rules on data interpretation.

Part III [*Pure Appl. Chem.* 1976, **45**, 105–123] deals extensively with the nomenclature of analytical flame (atomic emission and absorption) spectroscopy and associated procedures.

Part IV [*Pure Appl. Chem.* 1980, **52**, 2541–2552] concerns X-ray emission (and fluorescence) spectroscopy.

Part V [*Pure Appl. Chem.* 1985, **57**, 1453–1490] deals with the classification and description of radiation sources.

Part VI [*Pure Appl. Chem.* 1984, **56**, 231–345] covers molecular luminescence spectroscopy.

Part VII [*Pure Appl. Chem.* 1988, **60**, 1449–1460] is concerned with molecular absorption spectroscopy (UV/VIS).

Part VIII [*Pure Appl. Chem.* 1991, **63**, 735–746] deals with a new nomenclature system for X-ray spectroscopy.

Part IX [*Pure Appl. Chem.* 1995, **67**, 1725–1744] cov-

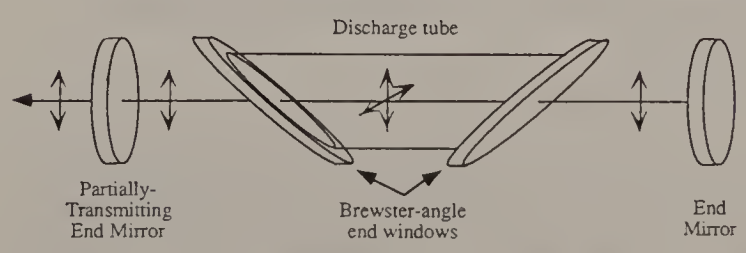


Fig. 1 Schematic representation of a gas laser cavity. Double-headed arrows indicate electric field polarization directions, and show the beam polarization produced using Brewster-angle end windows on the discharge tube.

ers fundamental aspects of spectral dispersion and isolation of radiation.

Part X [*Pure Appl. Chem.* 1988, **60**, 1461–1472] deals with sample preparation for analytical atomic spectroscopy and other related techniques.

Part XI [*Pure Appl. Chem.* 1995, **67**, 1745–1760] deals with the detection of radiation.

Part XII [*Pure Appl. Chem.* 1992, **64**, 253–259] deals with terms related to electrothermal atomization.

Part XIII [*Pure Appl. Chem.* 1992, **64**, 261–264] deals with terms related to chemical vapour generation.

A document on laser-based atomic spectroscopy is in the approval process.

This document, Part XV, deals with the fundamental properties of lasers used in laser-based molecular spectroscopy for chemical analysis. It complements parts I, V, VI, VII, IX and XI, and lays the ground work for Parts XVI (Luminescence), XVII (Absorption), XVIII (Raman Scattering Processes) and XIX (Photothermal Detection) of the series.

Basic aspects of lasers, types of lasers, principles of laser propagation, and details of the dynamical properties of lasers are covered, as used in molecular spectroscopy for chemical analysis. The spectral region considered ranges from 100 nm to 1 mm.

This Report was prepared for publication by D.S. Moore[1], T. Vo-Dinh[2], N.H. Velthorst[3] and B. Schrader[4] ([1]Chemical Science and Technology Division, Los Alamos National Laboratory, Los Alamos, NM 87544, USA; [2]Advanced Monitoring Development Group, Oak Ridge National Laboratory, Oak Ridge, IN 37831–6101, USA; [3]General and Analytical Chemistry, vnje Universiteit, De Boelalaan 1083, 1081 HV Amsterdam, Netherlands; [4]Institut fur Physikalische und Theoretische Chemie, Universitat-GH-Essen, D-45117 Essen, Germany) for the Commission on Spectrochemical and Other Optical Procedures for Analysis of the Applied Chemistry Division. Full details are to be found in Pure Appl. Chem. *1995, **67**, 1913–1928.*

Isotopic and nuclear analytical techniques in biological systems: A critical study—IX. Neutron activation analysis (Technical Report)

Synopsis: Neutron activation (NAA) methods applied to the analysis of biological samples are reviewed. Methods covered include instrumental neutron activation (INAA), prompt gamma NAA(PGNAA), radiochemical NAA(RNAA) and pre-irradiation separation methods (CNAA). The use of epithermal neutrons, fast neutrons, and applications to *in vivo* studies are also discussed.

Table 1 Detection limits (in g) by RNAA

10^{-9}–10^{-8}	10^{-10}–10^{-9}	10^{-11}–10^{-10}	10^{-12}–10^{-11}	<10^{-12}
Al Sn	Ba Nd Te	Sb I W	Au Re	Dy
Ca Ti	Cl Sc Tb	As Ga V	Ir Rh	Eu
Ce Y	Gd Se Th	Br La Yb	Lu Sm	Ho
Cd Zr	Ge Sr Tm	Cs Hg	Mn	In
Cr W	Hf Ta	Co Pd		
Mg		Cu Ru		
Mo		Er Na		

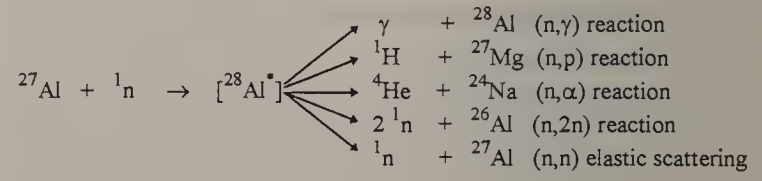

27Al + 1n → [28Al*]
γ + 28Al (n,γ) reaction
1H + 27Mg (n,p) reaction
4He + 24Na (n,α) reaction
2 1n + 26Al (n,2n) reaction
1n + 27Al (n,n) elastic scattering

Fig. 2 How Al may be detected using neutron activation.

This Report was prepared for publication by R.H. Filby (Department of Chemistry, Washington State University, Pullmann, WA 99164-4630, USA) for the Commission on Radiochemistry and Nuclear Techniques of the Analytical Chemistry Division. Full details are to be found in Pure Appl. Chem. *1995, **67**, 1929–1941.*

Isotopic and Nuclear Analytical Techniques in Biological Systems: A critical study—X. Elemental isotopic dilution analysis with radioactive and stable isotopes (Technical Report)

Synopsis: Isotope dilution is a method of chemical analysis based on the mixing (or dilution) of a radioisotope or a separated stable isotope with its natural isotope(s) in the sample. The activity ratio or isotopic ratio of the mixture defines the concentration of the analyte, which is a tremendous advantage for measurement since quantitative separation of the analyte is not required. The technique has a multitude of variations and has been combined with many classical and instrumental procedures used in analytical chemistry. The technique is noted for its accuracy. This review focuses on the application of the technique in the determination of elemental concentrations in biological systems.

This Report was prepared for publication by J.D. Fassett (National Institute of Standards and Technology, Technology Administration, Department of Commerce, Gaithersburg, MD 20899, USA) for the Commission on Radiochemistry and Nuclear Techniques of the Analytical Chemistry Division. Full details are to be found in Pure Appl. Chem. *1995, **67**, 1929–1941.*

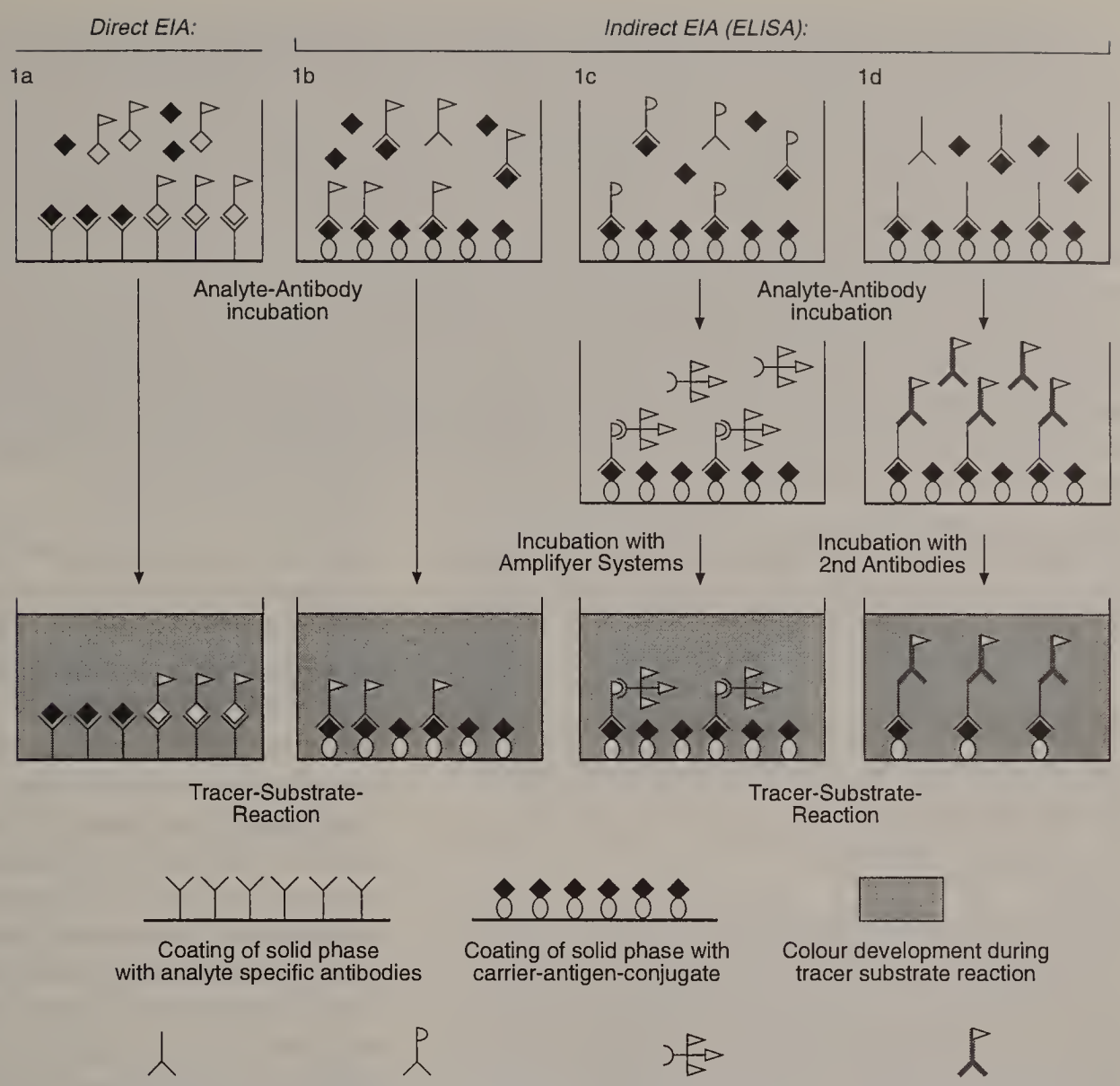


Fig. 1 Formats of direct and indirect, competitive immunoassay types.

Properties of EDAM copolymers as polypropylene resin modifier (Technical Report)

Synopsis: The use of a copolymer of ethylene and N,N′-diethylaminoethyl methacrylate (EDAM) when melt blended into polypropylene (PP) to improve the dyeing properties of propylene fibres has been studied. It has been shown that when EDAM was heated in air, the oxygen in air accelerates the thermal decomposition of the DAM moiety of EDAM at 150°C, leaving polyethylene as the residue. However, this heterogeneous reaction was not serious for the melt in extruder, in a capillary rheometer or in fibre spinning of PP/EDAM blends. Steady state viscosities of PP, PP/EDAM blends and EDAM under shear rates 10^0–10^4 s^{-1} at 200°C and first normal stress differences under shear stresses of 3.10^2–10^4 Pa at 200°C were measured.

Characteristics of the entrance flow to an orifice was measured using a die of length to diameter ratio $L/D = 0$ in a capillary rheometer to estimate the elongational flow effects of these melts. The rheological behaviour of PP/EDAM blends up to 20% EDAM resembles PP, while the PP/EDAM 50/50 blend resembles EDAM.

Transmission electron microscopy of microtomed sectons of the capillary extrudates of the PP/EDAM 80/20 blend and 50/50 blend showed clearly that the former has the morphology of EDAM islands in a PP sea while the latter the morphology of PP islands in an EDAM sea. For practical applications of EDAM-modified PP fibres, the EDAM content is less than 10%, such melt blends showed only a slight increase in viscosity. The dyeing behaviour of EDAM-modified PP fibres has also been studied. Two key chemicals which improve the dyeing properties of the EDAM-modified PP fibres were found. One of them is sodium stearate. When it is added to the PP/EDAM blends for spinning, it accelerates the penetration of dyestuff into the fibre. The other

is the potassium salt of an alkylphosphate to be used as a dyebath auxiliary which improves colour fastness and shows an antistatic finishing effect to the dyed fibre.

This report has been prepared for publication by R. Qian[1], Y. Xu[1], Y. Chen[1], D. Shen[1], X. Jin[1], L. Chen[1], T. Ohmae[2], S. Hosoda[2], H. Tanaka[2], T. Masuda[3], A. Nakajima[4] ([1]Institute of Chemistry, Academia Sinica, seijing 100080, China; [2]Chiba Research Laboratory, Sumitomo Chemical Co. Ltd, Chiba-ken 299–02, Japan; [3]Department of Materials Chemistry, Kyoto University, Yoshida, Sakyo-ku, Kyoto 606-ol, Japan; [4]Osaka Institute of Technology, Osaka 535, Japan), of the Working Party on Structure and Properties of Commercial Polymers from the Commission on Polymer Characterization and Properties of the Macromolecular Division. Full details are to be found in Pure Appl. Chem. *1995, **67**, 2047–2056.*

Major concerns and research needs for our understanding of the chemistry of the atmosphere (Technical Report)

Synopsis: Inputs of a questionnaire survey classified under the sections: global, regional/urban and indoor/workplace are presented. Major concerns and research needs for our understanding of the chemistry of the atmosphere are identified, together with suggestions for IUPAC's expected role in each of the three fields.

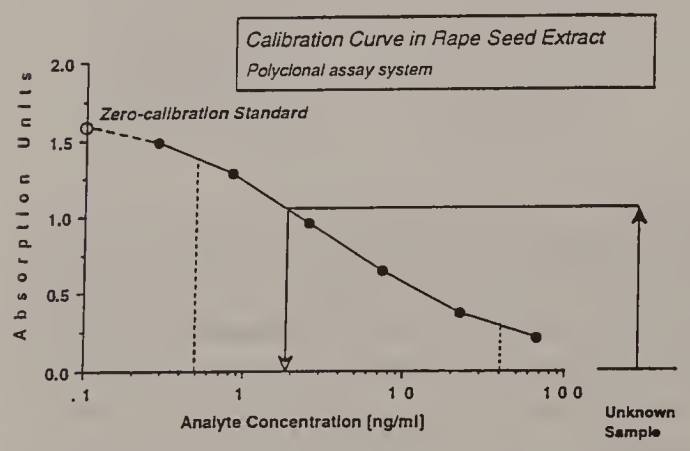


Fig. 2 Quantification of residues with ELISA assays.

This report has been prepared for publication by H. Akimoto (Research Centre for Advanced Science and Technology, The University of Tokyo, 4-6-1 Komaba, Mejuro-ku, Tokyo 153, Japan) of the Commission on Atmospheric Chemistry of the Applied Chemistry Division. Full details are to be found in Pure Appl. Chem. *1995, **67**, 2057–2064.*

Pesticides report 33. Immunoassays for residue analysis of agrochemicals: Proposed guidelines for precision, standardization and quality control (Technical Report)

Synopsis: Immunoassays (ELISA) for agrochemicals are analytical techniques which make use of antibodies as 'biochemical detectors' for the quantification of active ingredients or their derivatives. In contrast to clinical chemistry, the application of immunoanalytics to residue analyses of agrochemicals by industries, and the acceptance of ELISA data by registration agencies is still in its infancy. Missing performance quality control criteria for ELISAs in the past have raised questions about the reliability of this technique for the analysis of agrochemicals. This report gives basic technical information on immunoassays such as test formats and detection systems. Parameters critical for the reliabiliy of this methodology, such as matrix interference and cross reactivity, are discussed. Guidelines are proposed for precision requirements, standardized evaluation procedures and the distribution of immunoanalytical methods for agrochemicals. Follow-up activities are summarized with the intention of generating a wide database on the precision and applicability of irnmunoassays for agrochemical analysis.

This report has been prepared for publication by A.J. Krotzky[1] and B. Zeeh[2] ([1]BASF Corporation, Agricultural Research Centre, RTP, NC 27709-528, USA, [2]Agricultural Research Centre, BASF Akt., 67114 Limburgerhof, Germany) of the Commission on Agrochemicals of the Applied Chemistry Division. The full details are to be found in Pure Appl. Chem. *1995, **67**, 2065–2088.*

New publications

Szervetlen Kémiai Nevezéktan

A Hungarian translation of the *Red Book* (1990), *Nomenclature of Inorganic Chemistry*, has recently been published by the Hungarian Chemical Society. The original text has been adapted and translated by Piroska Fodorné Csányi and László Simándi. The publication was sponsored by the Chemical Section of the Hungarian Academy of Sciences (Magyar Tudományos Akadémia Kémiai Tudományok Osztálya), the Hungarian Chemical Society (Magyar Kémikusok Egyesülete) and the National Committe for

IUPACSEARCH Version 4.1

Free computer disks containing all IUPAC recommended nomenclature, symbols and technical reports published in *Pure and Applied Chemistry* from 1960 through to the end of 1994 are now obtainable from the IUPAC Secretariat.

The disks are 3½-inch, high-density, IBM-PC compatible format and will run under DOS (version 3.3 or later) or Windows. A hard disk with 5 Mb of free space and 640 Kb or greater of RAM are required. The software is easy to use, is menu-driven and allows for Boolean searches. Both colour and black and white monitors are supported. Sorry, a Macintosh version is not available.

Please E-mail or Fax your request to:

Mrs Gwyneth Pettit, Fax: +44 1943 880310; E-mail: acadsoft@bcs.org.uk

Technical Development (Országos Muszaki Fejlesztési Bizottság).

Anyone interested in obtaining a copy of this Hungarian translation of the Red Book should contact Dr Piroska Fodorné Csányi, Naphegy tér 5/b, H-1016 Budapest 1, Hungary.

Nomenclature on the World Wide Web

The first of several planned IUPAC nomenclature recommendations have been converted into a World Wide Web document which can be accessed from your desktop PC. The 'Glossary of class names of organic compounds and reactive intermediates based on structure. Recommendations 1995' [*Pure Appl. Chem.* **67**, 1995, 1307–1375] can now be consulted from: http://www.qmw.ac.uk/~ugca000/iupac.html. This document contains over 700 class names with over 1300 cross-links and 170 illustrations.

Due to the nature of the medium the material is now fully indexed and the entries are ordered into 22 categories so that related material is collated. The sections are: hydrocarbons, ring systems, alcohols and ethers, aldehydes and ketones, carboxylic acids, compounds with one nitrogen atom, compounds with more than one nitrogen atom, compounds containing boron, halogen, metals, phosphorus arsenic and antimony, silicon or germanium, sulfur, selenium and telurium, ions and radicals, natural products and miscellaneous entries. The natural products are subdivided into antibiotics, carbohydrates, lipids, nucleic acids, terpenoids, tetrapyrroles and other natural products.

Due to the limitations of the software used on the web, some characters have to be converted into text e.g. Greek letters are given as [alpha], etc. However, instead of just having a note that a term used in a definition is available elsewhere in the glossary there is now a link. Click on the word and the definition itself will appear.

In addition to the glossary there is a full list of nomenclature recommendations from the Commission on the Nomenclature of Organic Chemistry (III.1) and also for the Joint Commission on Biochemical Nomenclature, together with those of the Nomenclature Commission of the International Union of Biochemistry and Molecular Biology. There is also a link to the IUPAC page at Cambridge on the organization of the Union.

If you have any comments or suggestions please contact the author by E-mail: G.P.Moss@qmw.ac.uk

G.P. Moss, Department of Chemistry, Queen Mary & Westfield College, Mile End Road, London, UK.

IUPAC Series on Analytical and Physical Chemistry of Environmental systems. Volume 3, Metal Speciation and Bioavailability in Aquatic Systems

Most environmental systems are *living* systems in the basic sense: they are not immobile in thermodynamic equilibrium, but continuously *changing* thanks to the input of external energy (ultimately solar or geothermal). Such changes occur at all spatial (and time) scales, from the molecular level to the global scale, through micro and macroscales, e.g. in weathering processes which clearly encompass processes at all scales. Organisms, particularly micro-organisms, often play a dominant role in causing these changes, by generating different chemical reactions and conditions in different environmental niches (or compartments). This spatial diversity of chemical conditions may extend from a molecular to a macroscopic level and is generally organized into environmental *structures*. An obvious example is the assembly of soil horizons with various redox and acid-base properties; environmental systems include many other micro and macro structures. Finally, these different chemical conditions maintained in neighbouring compartments by the external input of energy, dictate the fluxes *of chemical compounds* between the compartments, either small or large.

A key feature of environmental chemistry is to understand and predict fluxes of vital and detrimental compounds. Hence the description of the various physical structures and of their chemical constituents as well as

their reactivity and environmental roles are key questions for investigation. This topic is dealt with in the first and the second volumes of this Series, namely *Environmental Particles*, Volumes 1 and 2 (ISBN 0 87371 589 6 and ISBN 0 87371 895 X, respectively), which describe colloids and biopolymers, in the nanometre to 100 μm range, their aggregation rates and structures, and their properties and environmental roles, in air, soils, waters and sediments. Two other volumes, specifically on air and soil particles, respectively, are in preparation. Solid–water interfaces, colloids and colloid aggregates however, are only a few examples of environmental structures. Other very important examples are sediment–water interfaces in lakes, rivers or oceans, air–water interfaces in soils, lakes and ocean, oxic–anoxic boundary layers in lakes or ground water, liquid–air interfaces in fog or rain droplets, soil porosity structure, etc. Not only is more information needed on these structures, but new analytical tools must be developed to study them in detail, without causing perturbations. A large number of recent techniques based on surface spectroscopies, electron microscopies, atomic force microscopies, light scattering, and many others, should be adapted to the specific needs of environmental sciences, for the description of the most important structures relevant to the functioning of ecosystems.

The second major issue of environmental chemistry is the determination of fluxes of (bio)-active compounds. Long-term biological productivity and diversity in environmental systems depend on compound fluxes at least as much as on their concentration. Estimation of pollution impacts therefore should not be based solely, as is done presently, on the analytical measurements made in the laboratory of compound concentrations in homogenized samples. The determination and study of fluxes is quite complicated. They result from the coupling of chemical kinetics and physical diffusion processes, often linked to rnicrobially catalysed transformation processes. The understanding of their origin therefore requires quantitative integration of chemical, physical and biological concepts. In addition, it is very difficult to reproduce, under controlled laboratory conditions, fluxes representative of natural systems; their experimental determination is complicated, both in the laboratory and *in situ,* because very steep gradients—occurring over submillimeter ranges—may affect ecosystems at the macroscale level. The development of specific analytical techniques for *in situ,* high resolution (submillimetre) concentration gradient measurements are therefore closely linked to the improvement of our knowledge of environmental processes, and is a major challenge for analytical chemistry in general.

Another specificity of environmental chemistry is the important role of chemical heterogeneity. Sediments, soils and aquatic colloidal material include an extremely large number of components, all of which may contribute to a different extent to a particular chemical property (acid–base, redox, complexation) of the target environmental system. The net result is an efficient buffering of the corresponding intensity parameter value (pH, redox potential, free metal ion), which plays a key role in maintaining the stability of biological ecosystems. However, the rigorous chemical description of these intensity parameters is quite complicated, since their value results from a weighted average of the contributions of all the constituents. In such cases, statistical approaches of chemical reactivity should be developed. Again, this physical chemistry problem is closely linked to an analytical challenge; indeed, the analytical tool necessary to determine environmentally meaningful intensity parameters based on well-defined weighting averages has yet to be developed.

A further important aspect is mathematical modelling. Understanding specific environmentally relevant physico-chemical reactions at the molecular or microscopic level would not be useful if it could not be coupled to other physical or biological processes. This is crucial in evaluating the overall behaviour of the ecosystem of interest, in making impact predictions, and in particular in evaluating the relative importance of the chemical processes. This is only feasible by means of numerical models. It is therefore of utmost importance that submodels, including detailed descriptions of the most relevant physico-chemical processes, be integrated into general macroscopic models of ecosystem behaviour. This is highly lacking at present.

The above discussion points out that the development of general predictive models enabling a correct evaluation of man's activities, requires detailed biophysicochemical studies, in particular in relation to structures and fluxes. Unfortunately, the traditional method for training chemistry students is still largely based on studies of homogeneous systems. Hence, students are not familiar with the techniques and concepts required for understanding physically heterogeneous systems, including processes encountered in other disciplines. This may be one of the reasons why environmental quality control is still largely based on the determination of total concentrations of compounds in homogenized samples, while speciation and fluxes would be key parameters for pollution evaluation.

The main purpose of this series is to make chemists and other scientists aware of the most important biophysico-chemical processes which influence the behaviour of environmental systems, in terms of sound quantitative theoretical concepts. The various volumes of this series emphasize processes which are specifically related to environmental systems, and which are often therefore unfamiliar to chemists with a main back-

ground in homogeneous reactions in solutions. The second major issue of this series is to discuss in parallel (either in the same book or in separate books) (i) the important bio-physico-chemical processes and structures discussed above, and (ii) the analytical tools which exist or should be developed to study them. As pointed out earlier, there is indeed a great need for methods developed specifically for this field in close connection with the corresponding process studies. We therefore feel that inclusion in the same series of both analytical aspects and process studies is essential. The development of specific analytical tools for molecular biology, biophysics, biochemistry and physiology has been carried out in parallel with the understanding of cell and organism functioning, and this has enabled great progress in this field. Similar tools are badly needed in environmental chemistry. It is hoped that this series will help promote this development, in order to deepen our knowledge of environmental biophysical chemistry.

J. Buffle and H.P. van Leeuwen
Series Editors

Metal contamination of aquatic ecosystems is a matter of concern to governmental authorities because it is widespread and because many metals are persistent and potentially deleterious to aquatic life. It is probable that our industrialized civilization will continue to produce metal wastes, at perhaps even increasing rates. The remediation of contaminated sites or reductions in waste disposal are possible but they are costly; the justification of such measures is usually difficult on the basis of present environmental quality criteria. It is clear that the development of rational, effective and economical strategies to solve the problems of contaminated environments will greatly depend on our ability to predict how remedial actions will improve environmental quality and how these changed conditions will affect aquatic organisms. The formulation of such predictive models presupposes an understanding of the geochemical and biological processes involved in trace metal bioaccumulation and in the manifestation of their toxic effects (Fig. 1).

Over the past 20 years substantial progress has been achieved in our understanding of metal interactions with aquatic organisms. In early studies designed to measure trace metal toxicity, solution chemistry was generally overlooked; oversaturated solutions, the uncontrolled complexation of trace metals, pH variations during experiments, adsorption and contamination by the labware, etc., were more the rule than the exception. Recent work has stressed the importance of controlling chemical speciation in the exposure medium external to the organism, i.e. the actual partitioning of the trace metal between the various ligands present. Bioassays performed in carefully controlled systems have revealed the central role played by free-metal ion activity, and this has led to the formulation of what is now known as the free-ion activity model. This awakening to the crucial role of solution chemistry gave rise to a strong interest in the development and use of both thermodynamic models to calculate the speciation of trace metals, and of analytical methods for speciation measurements. In parallel to these noteworthy chemical developments, important progress has also been achieved in our knowledge of metal detoxification mechanisms, the importance of food as a route of trace metal uptake, the transfer of metals along food chains and the role of various biological factors in metal accumulation in organisms.

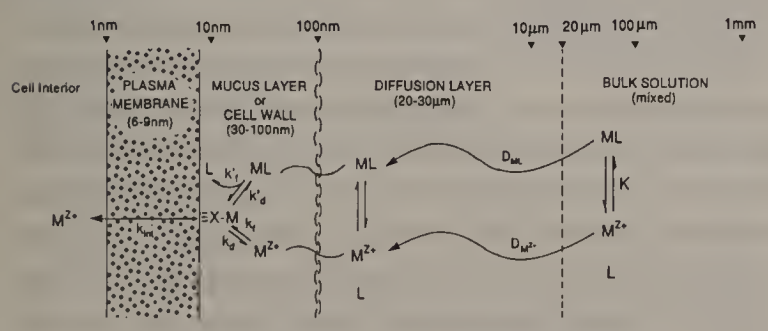


Fig. 1 Conceptual model of metal–organism interactions.

It is perhaps trite to point out that the study of trace metals interactions with aquatic organisms requires an interdisciplinary approach. An appreciation of the importance of the biological, biochemical, geochemical and chemical aspects involved is a prerequisite for studying trace metal–organism interactions; none of these aspects can be ignored. Therefore the main purpose of this book was to bring together specialists from various disciplines to cover—in a comprehensive and critical manner—various aspects of trace metal organism interactions. It was our intention to identify some of the assumptions and shortcoming of past research, and thus to provide some suggestions for future research.

The chapters of the book are organized in a rational fashion, so that the reader progresses from fundamental concepts and models to speciation measurements and field applications. Organisms are in contact with trace metals through their cell wall and plasma membranes. The accumulation of metals or the expression of their toxicity starts with their reaction at sites on the membrane and with their transport across the plasma membrane; the mechanisms of these processes are discussed in Chapter 1 . The free-ion activity model is often used to describe the uptake of trace metals by aquatic organisms and the manifestation of their toxic effects. Chapter 2 describes this model and summarizes the available literature supporting it for a variety of aquatic organisms; most of the apparent exceptions to the free-ion activity model are also rationalized, based

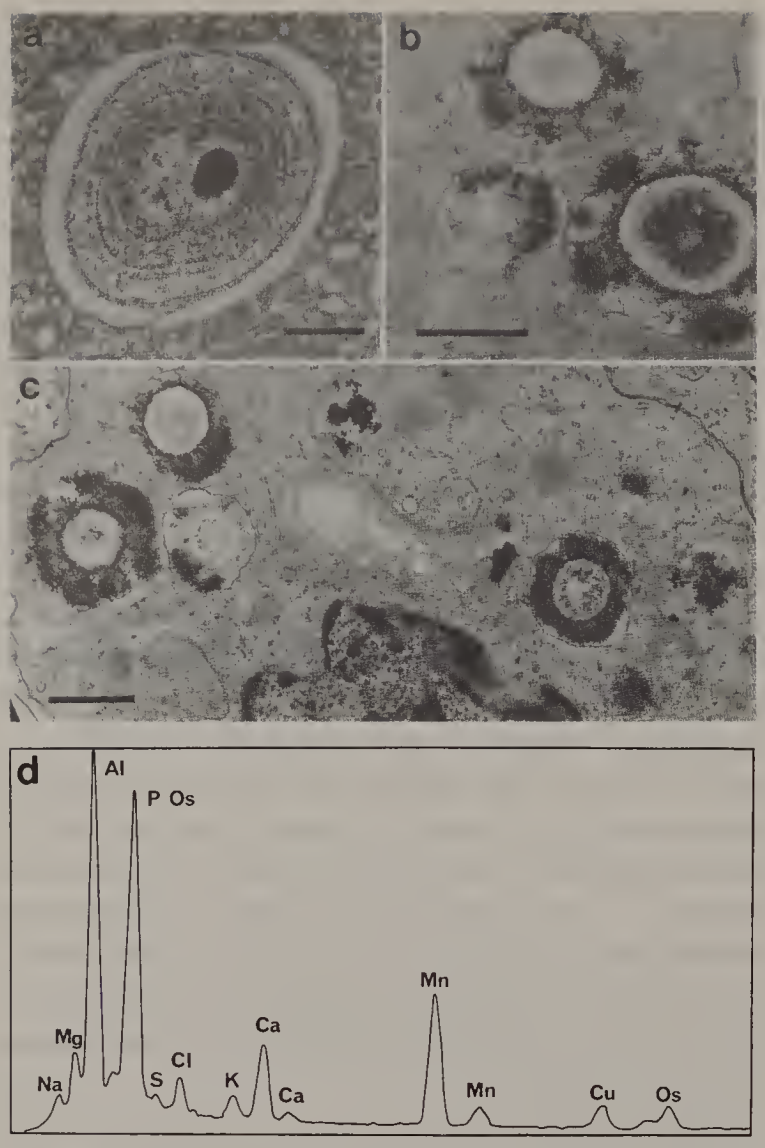


Fig. 2 Transmission electron micrographs of basophil cell granules from gastropod mollusks. Taken from Metal Detoxification in Aquatic Organisms, A.Z. Mason and K.D. Jenkins, chapter 10 of the present volume.

on the nature of the dissolved ligands and on the metal species formed at physiologically active sites at the plasma membrane. Chapter 3 focuses on organometals which, as a class, do not conform to the free-ion activity model.

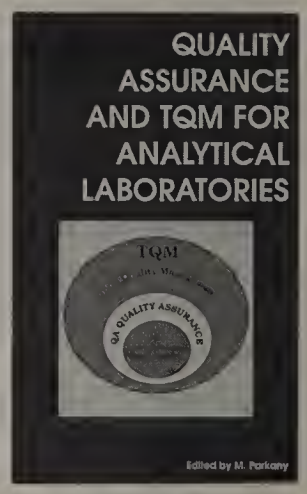
From Chapters 2 and 3 it is obvious that the effects of trace metals on aquatic organisms (accumulation, nutrition, toxicity) depend on metal speciation in the external environment. Chapter 4 considers the chemical complexity of natural waters and reviews the current status of the thermodynamic approaches to trace metal speciation, i.e. the calculation of the partitioning of trace metals on the basis of their total concentrations and the chemical composition of the medium. Three chapters then describe electrochemical (Chapter 5) and non-electrochemical (Chapter 6) methods for measuring labile chemical species and chromatographic methods (Chapter 7) for measuring non-labile species (Fig. 2).

Animals can potentially obtain trace metals from ingestion of food as well as from water; Chapter 8 examines the transfer of trace metals in food webs and its implications for trace metal cycling. In relating metal concentrations in organisms to environmental levels, it is necessary to take into account biological factors that contribute to the variability of trace metal concentrations in organisms at a given site; these aspects are critically reviewed in Chapter 9. Once trace metals enter the intracellular environment, they encounter a variety of ligands, and the binding of the metal to some of these ligands may perturb the normal cell metabolism. Chapter 10 discusses the mechanisms of metal toxicity and the detoxification strategies that organisms have developed to prevent metal toxicity; it also stresses the analytical problems associated with the intracellular metal speciation studies.

Many types of bioassays, ranging in complexity from individual organisms exposed to a single trace metal in a beaker, to manipulations of a whole lake ecosystem, have been used to study trace metal–organism interactions. Chapter 11 shows that bioassays have been very useful tools for understanding fundamental aspects of trace metal toxicity, but that extrapolation from laboratory experiments to nature is difficult. It also addresses the limitations of bioassay techniques that are often used as a basis for management decisions, for assessing damage to the natural environment and for predicting how changed environmental conditions will affect the ecosystem.

Metal Speciation and Bioavailability in Aquatic Systems is the third volume in the IUPAC Series on Analytical and Physical Chemistry of Environmental systems. This current volume is edited by André Tessier & David R. Turner. John Wiley & Sons, Chichester, UK, 1995; xv + 678 pp.; GBP 100; ISBN 0 471 95830 1.

Quality Assurance and Total Quality Management for Analytical Laboratories



The success of the Fifth ISO/IUPAC/AOAC Symposium in 1993 on Quality Assurance for Analytical Laboratories can be attributed to the many excellent papers which presented the state-of-the-art of the relevant technology at that time.

We would all agree that laboratory analysis is not an isolated action, but is in most cases a service for others, using: samples taken, reagents and instruments prepared or supplied. Within the laboratory, a team of individuals performs the tasks. They are expected to use the purest solvents, specified reagents, calibrated instruments, the correct procedure, etc. These are all indispensable elements of the quality control process, which is part of quality assurance. Total quality management (TQM) contains these elements, and more. It also contains the human element—the devotion, the culture—and even

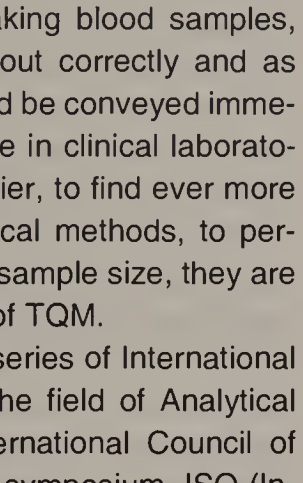
more. In fact, the boundaries of TQM cannot be fixed or closed. More and more new elements will be discovered that will expand what we mean by TQM.

In clinical laboratories, there are evident essentials of TQM. For example, not to confuse the samples, not to use contaminated needles for taking blood samples, etc. Analysis should be carried out correctly and as quickly as possible. Results should be conveyed immediately. Furthermore, when people in clinical laboratories strive to detect problems earlier, to find ever more faster and more accurate analytical methods, to perform the analysis from a reduced sample size, they are already responding to the ideals of TQM.

This volume is the sixth in the series of International Symposia for Harmonization in the field of Analytical Chemistry supported by the International Council of Scientific Unions (ICSU). For this symposium, ISO (International Organization for Standardization), IUPAC (International Union of Pure and Applied Chemistry) and NATA (National Association of Testing Authorities, Australia) combined their efforts to bring together in Australia approximately 30 lectures on the subject of Quality Assurance and Laboratory Management. ISO contributed to the Symposium with logistic help (e.g. printing and mailing the information leaflets, giving publicity to the Symposium, etc.) and also supplying the selected list of the relevant ISO International Standards and ISO/IEC Guides.

Quality Assurance and Total Quality Management for Analytical Laboratories, editor Michael Parkany. 1995, Royal Society of Chemistry; x + 288 pp.; GBP 47.50. ISBN 0 85404 760 3.

Phosphorus Cycles and Transfers in the Global Environment



Phosphorus (P) occupies a key place among nutrients because of its relative scarcity and its essential role in all life forms. Scientific information is increasingly needed to guide the use of P in order to obtain maximum benefits without producing undesirable impacts on the environment. The following Executive Summary provides the introduction for the scientific synthesis report resulting from the project on phosphorus cycling in terrestrial and aquatic ecosystems to be published in the SCOPE series in 1995. SCOPE launched this major study, chaired by Prof. C. V. Cole, in 1987. It sought to provide better understanding of the P cycle in terrestrial and aquatic ecosystems, and the global environmental effects of P. Regional workshops in Africa, Asia, Europe and South America synthesised data available in major ecosystems of each area considered and results were then integrated at an international workshop held in 1993 to provide a global perspective on the economic and environmental consequences of the use of P and recommendations and options for policy-planners and decision-makers. The project was supported by a number of public and private foundations and agencies whose assistance is gratefully acknowledged.

One result of synthesising the information gathered during the SCOPE project on 'Phosphorus cycles in terrestrial and aquatic environments' is the realisation that the term 'cycles' is not appropriate in the global context. It is estimated that currently 33 million tonnes per year of P are discharged into the oceans, while in 1990 16 million tonnes were applied as mineral fertilizer. The transfer to the oceans is largely the result of natural processes, which are accelerated by arable agriculture, concentrated animal husbandry and direct discharges from industry and domestic sewage. This publication therefore addresses P cycling and transformations in specific ecosystems, and also the less well understood transfers across landscapes and between ecosystems. A crucial problem in understanding the transfers from terrestrial to aquatic ecosystems is the great sensitivity of aquatic ecosystem function to P: the quantity of P sufficient to substantially alter the trophic status of a water body is negligible, and often not measurable, in the P budgets of terrestrial ecosystems in the watershed.

What are the processes that supply the essential nutrient P to the environment; and what is responsible for the oversupply that is threatening environmental integrity of aquatic ecosystems in some regions? In the natural environment, P is supplied through the weathering and dissolution of rocks and minerals with very low solubility. Therefore, P is usually the critical limiting element for plant and animal production, and throughout the history of natural production and human agriculture, P has been largely in short supply.

Many natural ecosystems and low-input farming systems have adapted to low P supply by recycling P from litter and soil organic materials. External P inputs have become available on a large scale with the mining of phosphate deposits and the wide-spread availability of the commodity 'phosphate'. This has de-coupled patterns of supply, consumption and waste production from natural nutrient cycles, and has made them dependent on economics. Although all continents show a positive P balance in their trade (excluding mined P deposits, which do not form part of the land ecosystems), P remains in short supply over large parts of the globe, where economic and political constraints mean that naturally low P availability's are only insufficiently supplemented by imported fertilizers.

Meanwhile, elaborate systems of fertility manage-

ment and a long history of P fertilizer use have built up soil P levels in developed countries to such an extent that additional P is not needed to produce food for the resident population. When such countries or regions continue to import both large amounts of animal feed and P fertilizers, and where populations are dense enough to produce significant amounts of waste phosphate, the P over-supply becomes a pollutant. In Europe, intensive animal production on farms with little land produces manure in excess of the nutrient requirements of crop and pasture lands. The excess P from the animal manure accumulates in the surface soils which leads to increased leaching and erosion losses of P to aquatic environments. Current legislation may not address this problem effectively, although legislation to reduce the land application of P exists and is being tightened with planned substantial reductions in allowable P application to soils, and stricter controls on timing and management. This trend has considerable impact on agricultural land use, and farmers are no longer solely regarded as producers of food but are also held responsible for the ecological functioning of the landscape. The stewardship required for intensive agricultural production that does not jeopardise the surrounding environment or the finite resources of rock phosphate, demands sophisticated methods of soil and landscape conservation, and nutrient management and monitoring.

Predicting the transformations, and therefore the potential for transfers from production sites to other ecosystems, of P requires detailed knowledge, not only of chemical equilibria but also of the rates of transformations of organic and inorganic forms of P in the soil, and of the ways in which P availability and turnover are affected by plant adaptations. Integrated farming systems, making use of biological processes of nutrient transformation and conservation and relying on long-term balancing of nutrient budgets, challenge the current knowledge base and the understanding of soil processes and management options. Knowledge has been integrated and extrapolated with computer models which evaluate soil, crop, management and climate information to optimise fertilizer application and permit the use of low-cost rock phosphates or recycled wastes.

A side effect of sustained heavy P fertilizer additions can be the accumulation and introduction into the human food chain of heavy metal contaminants contained in fertilizers. Phosphate fertilizer use has significantly increased soil cadmium levels. There are still no agreed safe Cd limits for soils, but it appears that concern about Cd build-up in soils may be warranted only where several critical factors combine, i.e. on acid soils with low cation exchange and low P fertility, to which significant P fertilisation is applied as low grade fertilizer or rock phosphate, particularly to Cd accumulators like leafy vegetable crops, and where the produce is the main source of local food consumption. This may be the case in truck farming belts around population centres in the tropics.

In developing countries, where 95% of the population increase over the next decades will occur, soil fertility is often low, and it will be difficult to meet the increased demand for food and fibre. The limited purchasing power of developing nations has resulted in nutrient mining of some of the better soils with the result that current productivity trends are downward. The limited use of fertilizer is compounded by the nearly complete use of high quality lands, which forces additional agricultural production into infertile acid upland soils. Too little fertilizer P is actually used in those parts of the world where P input could have a major effect on food production. Phosphorus use may have to double in Asia and quadruple in Africa. Fertilizer subsidies have been used in attempts to remedy this situation, but they can cause market distortions, black markets, environmental problems and the misallocation of resources. However, for reasons of long-term resource conservation and for the reversal of land degradation, fertilizer subsidies should be considered on P-deficient soils, where environmental costs of the soil resource depletion may justify the cost of subsidies. Careful monitoring of social and economic side effects would be required.

The development of acid upland soils, common in developing countries, requires the use of low-grade rock phosphate, which is less susceptible to leaching and fixation in the acid environment. As a result of logging and accelerated shifting cultivation accompanied by a rapid deterioration of soil fertility, an estimated 65–80 million hectares worldwide have been degraded into anthropic savanna and scrub. Reclamation of such degraded lands can be initiated by rock phosphate application which helps the establishment of legumes for nitrogen fixation and organic matter build-up. Subsequent management will have to be fine-tuned to release P from fertilizer in synchrony with crop demands.

Natural ecosystems on such acid soils usually conserve P in and recycle P from organic matter and plant residues. The rates of cycling of phosphorus, nitrogen and organic carbon are therefore closely inter-dependent, and must be viewed together if nutrient cycling and production dynamics are to be understood. Agricultural management can successfully mimic natural ecosystems, with—for instance—the use of mulches, green manure crops, legume covers, alley cropping and appropriate crop rotations. Much research and education are required to replace or adapt the originally successful regimes of shifting cultivation with such new technologies appropriate for increased food and fibre demands on a shrinking land base. Traditional farm communities passed on an intuitive feeling for nutrient dynamics, as expressed for example in the Norfolk ro-

tation or the intercropping patterns of the tropics. Extensive use of manufactured fertilizer has increased yields but has probably dulled this intuitive skill. Future generations of farmers will need to rediscover this knowledge to manage limited soil and fertilizer resources, aided by computer models and scientific knowledge that reduce the risks in farming diverse soils under variable climatic conditions. Many research results have not yet reached the farm level (e.g. use of mycorrhiza, the thorough understanding of nutrient cycles). This indicates that the linkage between scientists and farmers is not well established, training of farmers is insufficient, and feedback from farmers' problems to research is limited.

The lessons learned in managing a limited P resource under the economic constraints of developing countries may also benefit developed regions where P 'leaking' from production systems poses environmental threats. Fertilizer use to overcome P deficiency has permitted intensive sedentary agriculture which feeds large urban populations that now have waste P problems. Negative effects of P use are mostly associated with redistribution of P into aquatic environments where P limits bioproductivity and excess P increases the cycling of carbon, nitrogen and sulphur.

While the *in-situ* transformations of P, and their effects on C and N cycling are fairly well understood, the workshops have highlighted the complexity of P transfers in the landscape, and the lack of quantitative knowledge on landscape relationships. The P and N status of the world's major rivers reflects land use in their drainage basins, but the intricate relationships between land use patterns, surface and subsurface transport of P, and aquatic P loads are only now being explored. Because of their great sensitivity to P inputs, water bodies are a sensitive diagnostic for monitoring land use practices in the watershed. Point sources of P pollution from human population and industry add important P loads to surface waters, but these point sources are more easily controlled than diffuse sources. Reclamation and recycling of the P contained in industrial and urban waste waters is an important measure for pollution control. Although recycling is limited to some extent by heavy metal contamination, the problem is one of policy and engineering, which is not addressed in this volume.

In many aquatic ecosystems, non-point sources of P dominate the eutrophication process. Total P export rates from a watershed are related to arable land cover, slope, stream network density and rainfall, but the relationships are not strong enough to predict P exports to aquatic systems. Leaching and groundwater transport of P usually contributes less than 10% of the total P transport, the remainder being transported over the surface with runoff and erosion. Leached P, though, consists of soluble compounds with greater bio-availability and greater effects on eutrophication. Amounts of leached P are positively related to amounts of organic P and organic matter in the soil, and to P saturation resulting from over-fertilisation. P losses from soil erosion and surface runoff can range from 0.1–10 kg per hectare per year, or more on steep slopes. Mixed land use patterns of arable plots with forest fragments, meadows and pastures can halve total P export rates from watersheds. Afforestation belts, meadow strips, mid-field marshes, both natural and planted, are effective land use modifications effecting P retention.

Land margins of undisturbed vegetation belts or riparian zones bordering aquatic ecosystems act as filters for P and other nutrients, and also as catches for surface sediment runoff. Retention, particularly of soluble P is greatly influenced by the water balance of the ecosystem, and retained P may be re-released under reducing conditions or in organic forms. In situations of high nutrient loads, it may therefore be necessary to harvest P scavenger plants from riparian strips, or excavate P-saturated sediments and transport them back to the agricultural source site.

Watersheds cannot be managed only to control P transfers, and different management goals such as nutrient conservation, the accretion and/or conservation of soil organic matter and the maintenance of the biological diversity of ecosystems must be balanced. Environmental management should be based on a network of small-scale, 'closed' nutrient cycles associated with a variety of patches, spatially and temporally connected in the landscape by ecological flows. Control and prediction of nutrient movement may depend on the number, size, shape, sequence and configuration of patches in a landscape. This is a level of complexity well beyond current landscape-, erosion- and nutrient-cycling models. In addition to sophisticated models of P transport in landscapes, a simplified approach has therefore been developed, based on a susceptibility index using soil and site properties and management information.

Runoff, and to a lesser extent, groundwater move P to surface waters, which thus receive a mix of dissolved and particulate P. This mix varies greatly with the amount of sediment in runoff, and with storm intensity and duration. On average, surface waters contain 10 microgrammes per litre of soluble P, and suspended sediments carry 1000 µg/g. The average suspended sediment is therefore P-enriched relative to the source soils, and the solution P concentration is similar to that of average soil solutions, but higher than rain water. The resulting P exchanges between the solution and suspended or bed sediments greatly modify P bioavailability. Uptake of P by algae reduces solution concentrations, activating further exchanges. Eventually algae die, sediment out and/or re-release P for further uptake cycles. Algal growth due to P is the main

cause for eutrophication of inland waters, although cells or populations may exhibit N or P limitation, or switch between them. Cellular storage and population changes shift productivity limitations from one element to another, and introduce micro-scale and temporal variability. Therefore the solution composition of surface waters rarely reaches equilibrium, and is largely determined by the kinetics of processes.

The overall result of these processes depends on a mosaic of patches along streams and in lakes with different substrates and biota forming highly complex systems at micro- and meso-scales. The net result of increased primary productivity from excess P though is relatively simple to gauge: increased biomass and subsequent decomposition, which can lead to oxygen shortages, faunal death and reductions in water quality. Many of the factors discussed are exemplified in the basin study of Lake Balaton, Hungary, which receives river inflow, filtered through a constructed marsh, and direct runoff from the surrounding agricultural and urban landscape.

Fluvial transport of biologically active P adds up to about 2 million tonnes per year, all of which eventually reaches estuaries and coastal seas where eutrophication is an increasingly serious problem. Nitrogen appears to play a more important role in the eutrophication of coastal waters than P, but spatial variability is great. As freshwaters mix with tidal marine waters, both geochemical and biological conditions change rapidly, and complex nutrient limitations involving N, P and Si occur. Coastal biota such as corals, sea grasses and algal beds are particularly sensitive to increased nutrient inputs. Effects are aggravated by long residence time of water masses in deep channels, and continuous density stratification of the water caused by salinity gradients. The latter predispose the water mass to oxygen deficiency resulting from excess biological productivity. Because of the greater volumes over which biogeochemical processes are integrated in marine environments, laboratory and microcosm studies become difficult to apply. As a result, the reliability of data on nutrient cycles and limitations decreases from fresh water environments to estuaries, coastal seas and finally open oceans. Tropical mangroves serve as an example of the full complexity of P cycles and transfers at the terrestrial/aquatic interface. Here, fluvial P transport meets soils or sediments undergoing periodic flooding with both fresh and saline waters. Both terrestrial plants and aquatic organisms use and recycle this P. Mangroves, about whose P cycles relatively little is known, may therefore be an excellent proving ground for the methodology of study. Extractions of soils and sediments, speciation of water P, kinetics of physicochemical exchange and biological cycling and accretion in the long-lived biomass of mangrove trees, all play a role in the nutrient balance. The discussion of the mangrove ecosystem therefore also sheds some light on methodology as it applies and is used by the separate groups of aquatic and terrestrial scientists.

At the core of all the science and data presented are some real concerns about food security and environmental integrity. Some of these can be summarised in programmatic statements:

- Phosphorus is a major constraint on food and fibre production. Therefore, an economical supply of P is a necessity for a secure production in agriculture and forestry.
- An inefficient way to satisfy this P demand is by the exclusive use of inorganic fertilizers, which normally are expensive imports, and which often have relatively low-use efficiency in the field.
- Management and research must aim at nutrient and organic matter cycling in combination with sufficient fertilizer use to avoid 'nutrient mining' in agriculture and forestry.
- Regions which have a grossly positive P balance through the import of fertilizers and feed require political and legal mechanisms to (a) control land use patterns (b) avoid the decoupling of P discharges of animal production from the P requirements of plant production (c) manage landscapes in an integrated manner that avoids discharge to ground and surface waters (d) facilitate recycling of urban wastes through reducing heavy metal contamination.
- Eutrophic inland waters and their watersheds should be managed to limit P inputs, because P is easier to control than N, which can be entrained from the atmosphere.
- Coastal waters are increasingly suffering from high nutrient loads. Phosphorus is only part of their problem, and management will be complex. The sensitivity of some coastal ecosystems means that prevention should be favoured over damage management.
- The differences in the scientific approaches to terrestrial and aquatic ecosystems are ignoring some of the similarities between the systems. This might be remedied by more active dialogue between the disciplines. Certainly aquatic ecosystems are the recipient of nutrient losses from the land and should serve as indicators for the success (or lack of) of terrestrial P management.

SCOPE 54 – Phosphorus in the Global Environment, Transfers, Cycles and Management, edited by Holm Tiessen is published by John Wiley & Sons Ltd, Baffins Lane, Chichester PO19 1UD, UK. ISBN 0 471-95 691-0, price GPB 50.

Health and Safety Guides

The Environmental Health Criteria (EHC) monographs produced by the International Program on Chemical

Safety (IPCS) include an assessment of the effects on the environment and on human health of exposure to a chemical or combination of chemicals, or physical or biological agents. They also provide guide-lines for setting exposure limits.

The purpose of a Health and Safety Guide (HSG) is to facilitate the application of these guide-lines in national chemical safety programs. The first three sections in a HSG highlight the relevant technical information in the corresponding EHC. Section 4 deals with advice on preventive and protective measures and emergency action; health workers should be thoroughly familiar with the type of information found in this section. The section on regulatory information has been extracted from the legal file of the International Register of Potentially Toxic Chemicals (IRPTC) and from other United Nations sources.

Three new guides have recently been published, they are:

Health and Safety Guide no. 91, Isophorone (ISBN 92 4 151091 9)

Health and Safety Guide no. 92, Morpholine (ISBN 92 4 151092 7)

Health and Safety Guide no. 93, Brodifacoum (ISBN 92 4 151093 5)

Health and Safety Guide no. 94, Bromadiolone (ISBN 92 4 151094 3)

Health and Safety Guide no. 95, Difenacoum (ISBN 92 4 151095 1)

Health and Safety Guide no. 96, Warfarin (ISBN 92 4 151096 X)

Health and Safety Guide no. 97, Methomyl (ISBN 92 4 151097 8)

Health and Safety Guide no. 98, Chlorothalonil (ISBN 92 4 151098 6)

Health and Safety Guide no. 99, Diflubenzuron (ISBN 92 4 151099 4)

Published by the World Health Organization for the International Program on Chemical Safety. These publications are priced CHF5 in developed countries and CHF3.5 in developing countries. Further information and copies are available from, Distribution and Sales, World Health Organization, 1211 Geneva 27, Switzerland.

Macromolecular Symposia

Under the sponsorship of the International Union of Pure and Applied Chemistry (IUPAC), the International Conference on Liquid Crystal Polymers ('94 ICLCP) was held at the Twenty-First Century Hotel, Beijing, China, on 6–9 September 1994, co-organized by Chinese Chemical Society, National Natural Science Foundation of China, China Association for Science & Technology, Peking University and Tsinghua University. The conference provided a forum for scientists in the field of liquid crystal polymers (LCP) to meet and discuss their work, to exchange new ideas and information, and to anticipate the future of LCPs. One hundred and twelve papers written by 295 authors from 17 countries, were presented by about 100 scientists who participated in the conference. The programme included 17 invited lectures, 36 oral presentations and the posters.

The presentations dealt with molecular design and syntheses, characterization and structure, manufacturing and processing, composites, rheology and dynamics, theory and computer simulation, device physics and applications. The success of this conference was guaranteed by the presence of many noted scientists and by the high quality of the submissions.

The June 1995 issue of *Macromolecular Symposia* (Vol. 96) collected most of the invited lectures, together with a few selected contribution papers that were presented at the conference. There many notable contributions which included:

Structure and Dynamics of Liquid Crystalline Polymers with Different Molecular Architectures, by H. W. Spiess (Max-Planck-Institut für Polymerforschung, Posffach 3148, D-55021 Mainz, Germany).

Here, the structure and dynamics of liquid-crystalline polymers with different molecular architectures as revealed by multidimensional NMR are described. Specific examples discussed included semiflexible, rigid-rod, calamitic and discotic systems. Structural aspects addressed are the determination of high rank order parameters, the micro-order in frozen liquid crystals and the packing of flexible side chains. Local dynamics in the glassy state, conformational dynamics and collective phenomena such as the development of convective director structures were also discussed. It was demonstrated that advanced NMR spectroscopy yields highly specific information not available from conventional scattering, microscopic and relaxation techniques.

The liquid-crystalline behaviour of polymers can be an intrinsic property of rigid-rod macromolecules or it

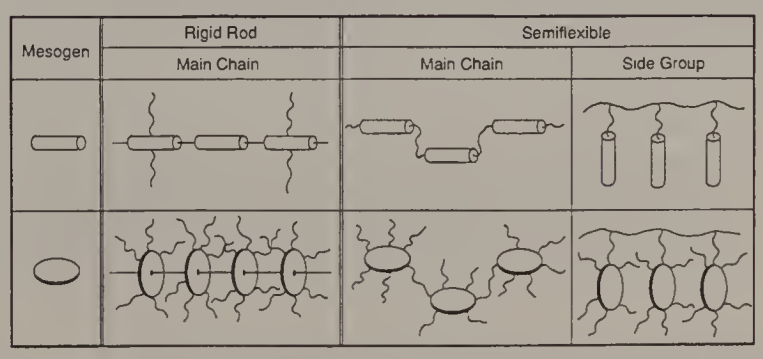


Fig. 1 Basic structures of liquid crystalline polymers.

can be induced by incorporating mesogenic units. The individual mesogens can be directly linked together to form rigid-rod systems or connected via flexible spacers to form semi-flexible systems. Moreover, the mesogens can be either incorporated into the main chain or attached as side groups to polymer chains to generate different types of liquid-crystalline polymers (LCP) as shown schematically in Fig. 1.

In order to relate the material properties of LCPs to molecular structure, the degree of alignment as well as the mobility of the different structural units must be determined. This calls for highly selective analytical tools like NMR. In fact, pulsed H-NMR of selectively deuterated systems has already provided a wealth of information about the structure and dynamics of these systems. In this overview, the author discussed advanced two-dimensional techniques that provide information about conformation, mobility and spatial proximity of different structural units. Such studies address a considerable variety of topics, including:

- Order parameters of different structural units;
- Micro-order in frozen liquid crystals;
- Local dynamics of mesogens in the glassy state;
- Conformational dynamics in the mesophase as well as in the glassy state;
- Collective dynamics leading to the complex director structures;
- Axial motion of discotic mesogens in columnar structures;
- Organization of main chain and side chains in rigid rod systems.

On one hand, these different aspects reflect the different molecular architectures resulting from the organization of differently shaped mesogens to form partially ordered liquid crystals. It is clearly shown that solid-state NMR often provides important information not available by other methods. Thus it complements more conventional techniques like microscopy, scattering and relaxation.

Solid-state NMR exploits anisotropic, angular–dependent interactions of nuclear spins with their surroundings, in particular magnetic dipole–dipole coupling of nuclei among themselves. This interaction leads to broad NMR lines covering *c.* 50 kHz for ^{1}H–^{1}H homonuclear coupling and *c.* 25 kHz for ^{1}H–^{13}C heteronuclear coupling. The anisotropy of the ^{13}C chemical shift results in powder patterns covering *c.* 15 kHz at a field strength of 7 T. In addition to these magnetic interactions, nuclei with spin $I > ½$ can also have electric quadrupole moments. These are subject to quadrupole coupling of the nucleus to the electric field gradient at the nuclear site. For ^{2}H ($I = 1$) in C–^{2}H bonds it leads to spectral splittings of *c.* 250 kHz. Since C–H bonds are common in LCPs, ^{2}H labelling is particularly useful.

If one of the above-mentioned couplings dominates, either because of its strength or because the others have been suppressed by decoupling, the angular dependence of the NMR frequency in high magnetic fields can be expressed by a single equation applicable to all the couplings as:

$$\omega = \omega_L + 0.5\,\Delta(3\cos^2\theta - 1 - \eta\sin^2\theta\cos 2\varphi). \qquad (1)$$

Here ω_L is the Larmor frequency including isotropic chemical shifts, Δ describes the strength of the anisotropic coupling: i.e. anisotropic chemical shift or ^{3}C–^{1}H dipole-dipole coupling for ^{13}C, quadrupole coupling for ^{2}H, and η is the asymmetry parameter describing the deviation of the anisotropic coupling from axial symmetry ($0 \le \eta \le 1$). The angles θ, ϕ are the polar angles of the magnetic field B_o in the principal axes system of the coupling tensor. This in turn is often simply related to the molecular geometry. The unique axis of the coupling usually coincides with a bond direction, e.g. in heteronuclear dipole-dipole coupling it is along the ^{13}C–^{1}H bond, in ^{2}H quadrupole coupling it is along

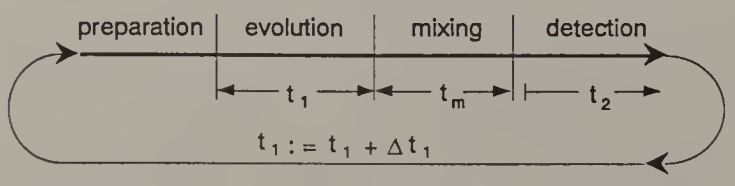


Fig. 2a Basic scheme of two dimensional NMR spectroscopy.

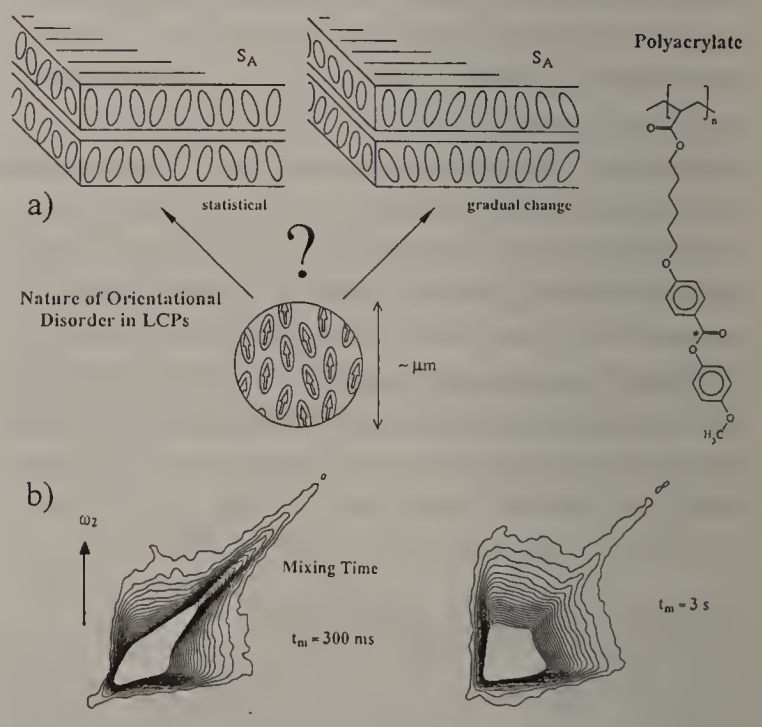


Fig. 2b Micro-order in frozen liquid crystalline polymers; (a) Schematic representation of nature of solid state disorder; (b) 2D exchange NMR spectrum of a smectic polyacrylate showing spin diffusion between ^{13}C in carbonyl groups with different orientations. The molecular structure of the system under investigation is shown on the right—the asterix marking the location of the position of ^{13}C enrichment.

the C–^{2}H bond, in ^{13}C chemical shift tensors of aromatic rings or carbonyl groups it is perpendicular to the sp^2 plane Depending on the total spin quantum number of the system, signals described by Eqn 1 and their mirror images with respect to ω_L may be superimposed. Moreover, in powder samples the individual spectra arising from all orientations of the coupling tensor are averaged to yield the powder lineshape. If the sample is partially ordered, e.g. in an aligned LCP, then the solid state NMR line shape reflects the orientation distribution function. Likewise, in presence of molecular dynamics, the solid-state spectrum is motionally narrowed and the degree of motional narrowing reflects the dynamic process involved.

Details of the experiments designed to record multidimensional NMR spectra were not given, since ample literature exists elsewhere on the subject. However, a two-dimensional (2D) NMR spectrum is generated by recording a two-dimensional data set following pulsed irradiation as a function of two time variables as shown schematically in Fig. 2, and subsequent double Fourier transformation. The development of the nuclear spin system in the *evolution period* with incremented time t_1 at the beginning of the pulse sequence provides the basis for the first frequency dimension ω_1. The NMR signal is detected in the *detection period* with time t_2 at the end of the pulse sequence, providing the basis for the second frequency dimension ω_2. In exchange *experiments,* a variable mixing *period* of duration t_m, during which dynamic processes can take place, is inserted between evolution and detection. In this way slow molecular dynamics are probed in real time. The concept of 2D spectroscopy is readily extended to three and higher dimensions by inserting additional evolution and mixing times.

The different molecular architectures resulting from the organization of the various liquid-crystalline polymers in their respective mesophases involve numerous questions about dynamic processes. This survey of the studies performed over several years clearly demonstrates that advanced multidimensional solid state NMR spectroscopy provides detailed information, not only on local molecular dynamics. It also can detect collective phenomena in liquid crystals such as the development of convection rolls and cooperative axial motions in discotics.

Moreover, multidimensional solid state NMR provides details about the packing arrangements of the mesogens in frozen liquid-crystalline systems as well as high rank order parameters for individual structural elements. In most cases this detailed information is not available by other techniques. It is needed, however, in order to relate the molecular organization and behaviour in these partially ordered systems to their often unique material properties.

Another paper of interest was:

Cross-linkable vs. linear liquid-crystalline copolyesters, by J. Economy (University of Illinois at Urbana, USA).

During the past 25 years there has been considerable effort directed at the development of the liquid- crystalline, aromatic copolyesters (LCP) based on *p*-hydroxybenzoic acid (PHBA). A number of companies have introduced several compositional variations of the original Ekkcel (Xydar) system which consisted of the copolymer of PHBA and biphenol terephthalate. More recently, considerable work has been carried out to elucidate some of the unique features of these copolyesters. Some of the most interesting results have emerged from an examination of the high temperature chemistry of these materials. Thus, it has been shown that at very high temperatures of over 400°C the aromatic polyesters undergo very rapid interchain transesterification reactions (ITR) (1000/chain/10 seconds). For example, the homopolymer of PHBA at 450°C reacts within seconds with poly(2,6-hydroxynaphthoic add) (PHNA) to form the random copolymer. On the other hand, annealing the random copolymers of PHBA and PHNA near their crystal nematic transition results in a 50–70°C increase in the crystal-nematic transition temperature T_{CN}. This process is best interpreted as a partial ordering of the sequence distribution. The partially ordered PHBA/PHNA has also been shown to display an unusual low temperature degradation reaction most likely related to a thermal Fries reaction.

Our recent studies have built on this new knowledge of the high temperature ITR to explore the use of LCPs as adhesive bonds between two metal substrates. Thus, it has been shown that thin coatings of LCPs on metal substrates not only provide outstanding protection against corrosive environments but also will form a reasonably strong adhesive bond when heated under pressure in contact with another coated specimen.

An unusual extension of ITR has very recently been reported wherein thin films of cross-linked aromatic copolyesters have been shown to form a strong adhesive bond at elevated temperatures. The oligomeric precursors to these cross-linked resins are low melting solids which greatly facilitate processing into thin coatings. Use of these crosslinkable systems as adhesives, matrices for composites and as structural foams has been successfully demonstrated. A unique feature of these crosslinked aromatic copolyesters is the ability to recycle them for reuse as oligomers by high-temperature treatment with controlled amounts of acetic acid.

Conferences

XVIII International Carbohydrate Symposium, Milan, Italy, 21–26 July, 1996

IUPAC SPONSORED

The scientific programme of the XVIII International Carbohydrate Symposium will cover all aspects of the structure, synthesis, biochemistry, biotechnology, and industrial applications of monosaccharides, oligosaccharides, polysaccharides, and glycoconjugates, including nucleosides and nucleotides.

The symposium will consist of plenary lectures, a thematic plenary session, parallel sessions with invited lectures, and free communications which will be presented as posters. An limited number of papers will be selected from amongst the free communications to be delivered orally. The conference language will be English.

Topic A: Structure
Primary structure, conformational analysis, spectrochemical methods and analysis applied to carbohydrates, carbohydrate polymers and glycoconjugates.

Topic B: Synthesis
New methods of synthesis of carbohydrates and carbohydrate-containing biomolecules (antibiotics, nucleosides, nucleotides, glycoconjugates); use of carbohydrates as chiral synthons.

Topic C: Biochemistry
Various biological and medical aspects of carbohydrates and glycocojugates.

Topic D: Biotechnology and Industry
Biotechnological aspects of carbohydrate chemistry and biochemistry. Uses of carbohydrates in food, cosmetic, pharmaceutical and other industries.

The registration fee is 800 000 ITL for active participants, 450 000 ITL for students, and 200 000 ITL for accompanying persons.

For further information, please contact:

Dr Annamaria Naggi, Scientific Secretary, Istituto G. Ronzoni, Via G. Colombo 81, 20133 Milano, Italy. Tel.: +39 2 2364 187.

XVIIth International Conference on Organometallic Chemistry, Brisbane Conference and Exhibition Centre, Brisbane, Australia, 7–12 July, 1996

IUPAC SPONSORED

This conference will feature plenary and section invited lectures, oral presentations and poster contributions. It is planned to run three concurrent sessions dealing broadly with:

(i) Transition metal and 4f-metal organometallic compounds
(ii) Main group organometallic compounds
(iii) Metal compounds in organic synthesis and catalysis

and encompassing interdisciplinary topics such as:

- Environmental chemistry
- Industrial chemistry
- Materials chemistry

The registration fee is 850 AUD (650 AUD for a member of the Royal Australian Chemical Institute or a member of another kindred national chemical society) for active participants, 400 AUD (300 AUD for a member of the Royal Australian Chemical Institute or a member of another kindred national chemical society) for students, and 150 AUD for accompanying persons.

For further information, please contact:

XVIIth International Conference on Organometallic Chemistry, Faculty of Science and Technology, Griffith University, Brisbane QLD 4111, Australia. Tel.: +61 (0) 7 3875 7217; Fax: +61 (0) 7 3875 7656; E-mail: icomc@sct.gu.edu.au

XIVth International Symposium on Medicinal Chemistry, Maastricht, the Netherlands, 8–12 September, 1996

IUPAC SPONSORED

This conference will feature plenary and section invited lectures, oral presentations and poster contributions. It is planned to run three concurrent sessions dealing broadly with:

- Cardiovascular agents
- Chiral synthesis
- Pro-drugs

- Proteases in drug design
- Combinatorial chemistry
- Lipid lowering agents
- CNS agents
- Protein kinases and their signalling pathways
- Problems and progress in antibacterial and antifungal drug discovery
- Antiinfective agents
- Cytochrome P450
- Computational chemistry

The registration fee is 1050 NLG before 1 June 1996, 1200 NLG after 1 June 1996, for active participants; 525 NLG before 1 June 1996, 600 NLG after 1 June 1996, for students; and 250 NLG for accompanying persons.

For further information, please contact:

Van Namem & Westerlaken Congress Organization Services, PO Box 1558, 6501 BN Nijmegen, the Netherlands. Tel.: +31 24 323 4471; Fax: +31 24 360 1159

Seventh International Harmonization Symposium on the use of Recovery Factors, Orlando, Florida, USA, 4–5 September, 1996

The use of recovery factors is a controversial issue amongst analytical chemists. The objective of the current harmonization project is to bring together the various approaches used to compensate for analyte loss and make a recommendation as to the 'best practice.' Such a recommendation could be referenced and promoted by the various organizations interested in analytical methods.

For further information, please contact:

Dr Michael Parkany, ISO Central Secretariat, Case Postal 56, CH-1211 Genève 20, Switzerland. Tel.: +41 22 749 0111; Fax: +41 22 733 3430.

110th AOAC INTERNATIONAL Annual Meeting and Exposition, Orlando, Florida, USA, 8–12, September, 1996

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Topics to be discussed include:

- Reliability of immunoassays;
- Technological society at risk—Problems in analyst training;
- Mycotoxins;
- Microbiological analysis—*Cryptosporidium*;
- ISO 9000 and 25—Do we need either?;
- Antibiotic residues in food;
- Advances in capillary electrophoresis;
- Methods for detecting pesticides;
- Methods for detecting beta-agonists;
- Pathogenic bacteria and their toxins—Using commercial test kits;
- Complex carbohydrates;
- Biological significance of animal drug and pesticide residues in food;
- Antibiotics and drugs in feeds forum;

For further information, please contact:

AOAC Meetings Department, 481 North Frederick Avenue, Suite 500, Gaithersberg, MD 20877-2504, USA. Tel.: +1 301 924 7077; Fax: +1 301 924 7089; E-mail: aoac@aoac.org

Conference Calendar

1996

Molecular order in polymers

21–24 May

2nd International Symposium on Molecular Order and Mobility in Polymer Systems. St. Petersburg, Russia.

Academy of Sciences, Bolshoy pr. 31, St. Petersburg, 199004 Russia

Free-radical polymerization

26–31 May

2nd International Symposium on Free-Radical Polymerization: Kinetics and Mechanism. Santa Margherita Ligure, Genoa, Italy.

Prof. S. Russo, Department of Chemistry, University of Sassari, Via Vienna 2, I-07100 Sassari, Italy. Tel.: +39 (79) 229556; Fax: +39 (79) 229559.

Mycotoxins and phycotoxins

27–31 May

9th International Symposiums on Mycotoxins and Phycotoxins. Rome, Italy.

Dr Marina Miraglia, Instituto Superiore Sanità, Food Department, Viale Regina Elena, 299, I-00161 Rome, Italy. Tel.: +39 (6) 4990, ext. 377; Fax +39 (6) 4451767.

Protein folding

17–20 June
International Symposium on Theoretical and Experimental Aspects of Protein Folding. San Luis City, Argentina.
Dr J. Vila, IMASL-Universidad Nacional de San Luis, Ejército de Los Andes 950, 5700 San Luis, Argentina.

Oxidation of polymers

24–28 June
11 International Conference on Polymers 'Thermal and Photo-Induced Oxidation of Polymers and its Inhibition in the Upcoming 21st Century'. High Tatras, Slovak Republic.
The Organizing Committee of the 11th Bratislava International Conference on Polymers, Polymer Institute of the Slovak Academy of Sciences, Dúbravská cesta, 842 36 Bratislava, Slovak Republic.

Surface forces

25–29 June
11th International Conference on Surface Forces. Moscow, Russia.
Dr L. B. Boinovich, Institute of Physical Chemistry, Leninsky Prospect 31, 117915, Moscow, Russia.

Organic synthesis

30 June–4 July
11th International Conference on Organic Synthesis. Amsterdam, Netherlands.
Conference Secretariat ICOS—11, PO Box 1558, 6501 BN Nijmegen, Netherlands. Tel.: +31 (80) 234471; Fax: +31 (80) 601159.

Catalysis

30 June–5 July
11th International Congress on Catalysis. Baltimore, USA.
Prof. Gary L. Haller, Department of Chemical Engineering, Yale University, PO Box 208286, New Haven, CT 06520-8286, USA. Tel.: +1 (203) 432 4378; Fax: +1 (203) 432 4387.

Organometallic chemistry

7–12 July
17th International Conference on Organometallic Chemistry. Brisbane, Australia.
Prof. C. Raston, Department of Chemistry, Monash University, Clayton, VIC 3168, Australia.

Chemical education

14–19 July
14th International Conference on Chemical Education—Chemistry: Expanding The Boundaries. Brisbane, Australia.
Dr W. Beasley, Graduate School of Education, The University of Queensland, Brisbane, Queensland 4072, Australia.

Sweeteners

14–20 July
International Symposium on Sweeteners. Jerusalem, Israel.
International Symposium on Sweeteners, PO Box 50006, Tel-Aviv 61500, Israel. Tel.: +972 (3) 5140014; Fax: +972 (3) 5175674 or 5140077; E-mail: 100274.2665@compuserve.com

(Bio)degradable polymers

15–18 July
37th Microsymposium on Macromolecules (Bio)degradable Polymers: Chemical, Biological and Environmental Aspects. Prague, Czech Republic.
Dr B. Valter, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám 2, 162 06 Prague c-Petriny, Czech Republic

Carbohydrates

21–26 July
18th International Carbohydrate Symposium. Milan, Italy.
Prof. B. Casu, Istituto di Chimica é Biochimica 'G Ronzoni', via G. Colombo 81, 20133 Milan, Italy.

Photochemistry

21–26 July
16th Symposium on Photochemistry. Helsinki, Finland.
Prof. J. Wirz, Institut für Physikalische Chemie, Universität Basel, Klingelbergstr. 80, CH-4056 Basel, Switzerland.

Solubility phenomena

22–25 July
7th International Symposium on Solubility Phenomena. Leoben, Austria.
Prof. H. Gamsjäger, Chairman 7th ISSP, Institut für Physikalische Chemie, Montanuniversität Leoben, Franz-Josef-Strasse 18, A-8700 Leoben, Austria.

Macromolecules

4–9 August.
36th International Symposium on Macromolecules. Seoul, Republic of Korea.
Dr Kwang Ung Kim, Secretariat of IUPACMACRO SEOUL'96, Division of Polymers, Korea Institute of Science & Technology, PO Box 131 Cheongryang, Seoul 130-650, Korea. Tel.: +82 (2) 957 6104; Fax: +82 (2) 957 6105; E-mail: iupac@kistmail.kist.re.kr

Excitonic processes

14–17 August
2nd International Conference on Excitonic Processes in Condensed Matter (EXCON '96). Bad Schandau, Saxonia, Germany.
Prof. M. Schreiber, Faculty of Natural Sciences, Technische Universität Chemnitz-Zwickau, D-09107 Chemnitz, Germany.

Coordination chemistry

18–23 August
31st International Conference on

Coordination Chemistry. Vancouver, Canada.
31st ICCC Secretariat, UBC Conference Centre, 5961 Student Union Boulevard, Vancouver, BC, Canada V6T 2C9. Tel.: +1 (604) 822 1050; Fax: +1 (604) 822 1069.

Macromolecular condensed state

20–25 August
International Symposium on Macromolecular Condensed State. Beijing, China.
Prof. Xibai Qiu, Secretariat, ISMCS "96, Chinese Chemical Society, PO Box 2709, Beijing 100080, China. Tel.: +86 (1) 0256 8157 or 0256 4020; Fax: +86 (1) 0256 8157; E-mail: qiuxb@infoc3.icas.ac.cn

Physical organic chemistry

25–29 August
13th International Conference on Physical Organic Chemistry. Seoul, Republic of Korea.
Prof. J. Suh, Department of Chemistry, Seoul National University, Seoul 151–742, Republic of Korea. Tel.: +82 (2) 8862184; Fax: +82 (2) 8743704; E-mail: jhsuh@plaza.snu.ac.kr

Biotechnology

25–30 August
10th International Biotechnology Symposium. Sydney, Australia.
10th IBS '96 Symposium Secretariat, GPO Box 128, Sydney, NSW 2001, Australia. Tel.: +61 (2) 262 2277; Fax: +61 (2) 262 2323; E-mail: veckels@tourhosts.com.au

Chemical thermodynamics

25–30 August
14th IUPAC Conference on Chemical Thermodynamics. Osaka, Japan.
Prof. M. Sorai, Executive Secretary of ICCT-96, Microcalorimetry Research Centre, Faculty of Science, Osaka University, Toyonaka, Osaka 560, Japan. Tel.: +81 (6) 850 5523; Fax: +81 (6) 850 5526 (or 5288); E-mail: icct96@chem.sci.osaka-u.ac.jp

Environmental biotechnology

1–4 September
International Conference on Environmental Biotechnology. Palmerston North, New Zealand.
Conference Secretary, Environmental Biotechnology Conference, Process & Environmental Technology Department, Massey University, Palmerston North, New Zealand. Tel.: +64 (6) 350 5351; Fax: +64 (6) 350 5654; E-mail: g.f.withers@massey.ac.nz

CHEMRAWN IX

1–6 September
Sustainable Production, Use, Disposal and Recycling of Materials. Seoul, Korea.
Organizing Committee & Secretariat, IUPAC CHEMRAWN IX, Tongwon B/D 6th Floor, 128-27 Tangju-dong, Chongno-ku, Seoul 110–071, Korea.

Euroanalysis IX

1–7 September
Euroanaysis IX. Bologna, Italy.
Prof. L. Sabbatini, Dipartimento di Chimica, Università di Bari, Via Orabona 4, 70126 Bari, Italy. Tel.: +39 (80) 544 2020/16/14; Fax: +39 (80) 544 2026.

Medicinal chemistry

8–12 September
14th International Symposium on Medicinal Chemistry. Maastricht, Netherlands.
Van Namen & Westerlaken Congress Organization Services, PO Box 1558, 6501 BN Nijmegen, Netherlands. Tel.: +31 (24) 323 4471; Fax: +31 (24) 3601159.

Food packinging

11–13 September
International symposium on Food Packaging: Ensuring Safety and Quality of Foods. Budapest, Hungary
Dr Laura Contor—ILSI Europe, Avenue E. Mounier, 83- Box 6, B-1200 Brussels, Belgium. Tel.: +32 (2) 7710014; Fax: +32 (2) 7620014.

Characterization of porous solids

15–18 September
4th International Symposium on Characterization of Porous Solids (COPS-IV). Bath, UK.
Elaine Wellingham, Conference Secretariat, Field End House, Bude Close, Nailsea, Bristol, BS19 2FQ, UK. Tel.: and Fax: +44 (1275) 853311.

Chemistry of natural products

15–20 September
20th IUPAC Symposium on the Chemistry of Natural Products. Chicago, USA.
IUPAC Symposium Headquarters, 5999 Butterfield Road, Hillside, Chicago, Illinois 60161, USA. For further information see http://www.a2z.com/iupac20/index.html

Multiphoton processes

30 September–4 October
7th International Conference on Multiphoton Processes. Garmisch Partenkirchen, Germany.
Prof. P. Lambropoulos, Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, D-85748 Garching, Germany.

Step growth polymerization

End-September
International Symposium on Step Growth Polymerization, Related Processes and Materials. Paris, France.

Dr B. Sillion, Laboratoire de Chimie Macromoléculaire, Université Pierre et Marie Curie, 4 place Jussieu, 75252 Paris Cédex 05, France. Tel.: +33 (1) 78 02 20 78; Fax: +33 (1) 78 02 20 10.

Pesticide use and environmental safety

14–17 October
International Workshop 'Pesticide Use and Environmental Safety in Latin America'. Sao Paulo, Brazil.
Dr K. Racke, DowElanco, 9410-North Zionsville Road, Bldg. 306-AZ, Indianapolis, IN 4628-1053, USA.

Mössbauer Effect

4–8 November
International Symposium on the Industrial Application of the Mössbauer Effect. Johannesburg, South Africa.
Prof. H. Pollak, Mössbauer Laboratory, University of the Witwatersrand, Private Bag 3, Johannesburg, WITS 2050, South Africa. Tel.: +27 (11) 7164051; Fax: +27 (11) 3398262; E-mail: isiame@physnet.phys.wits.ac.za

1997

Thermodynamics

5–8 January
International Symposium on Chemical and Biological Thermodynamics. Amritsar, India.
Prof. D. V. S. Jain, Department of Chemistry, Panjab University, Chandigarh 160014, India. Tel.: +91 (172) 541435; Fax: +91 (172) 541409; E-mail: dvs-jain@imtech ernet.in

Safety in Chemical Production

13–17 April
3rd IUPAC Workshop on Safety in Chemical Production: Environmentally Sustainable Manufacture of Competitive Products. San Francisco, USA.
Dr A. M. Ford, Gulf Coast Hazardous Substance Research Center, Lamar University, PO Box 10613, TX 77710-0613, USA. Tel.: +1 409 880 8768; Fax: +1 409 880 2397.

Bioorganic chemistry

1–6 June
4th International Symposium on Bioorganic Chemistry. Biarritz, France.
Prof. A. Marquet, Université Paris URA CNRS 493, Laboratoire de Chimie Organique Biologique, Tour 44/45-4 Pl. Jussieu, 75252 Paris Cedex 05, France.

Recycling of polymers

14–17 July
38th Microsymposium on Macromolecules, Recycling of Polymers. Prague, Czech Republic.
P.M.M. Secretariat, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám 2, 162 06 Prague c-Petriny, Czech Republic. Tel.: +42 (2) 36 0341; Fax: +42 (2) 36 7891; E-mail: sympo@imc.cas.cz

Interfacial phenomena

21–24 July
17th Discussion Conference on Macromolecules surface and interfacial phenomena in Macromolecular Systems. Prague, Czech Republic.
P.M.M. Secretariat, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám 2, 162 06 Prague c-Petriny, Czech Republic. Tel.: +42 (2) 36 0341; Fax: +42 (2) 36 7891; E-mail: sympo@imc.cas.cz

Bioinorganic chemistry

27 July–1 August
8th International Conference on Bioinorganic Chemistry. Yokohama, Japan.
Prof. M. Hidai, Department of Chemistry & Biotechnology, Graduate School of Engineering, The University of Tokyo, Hongo, Tokyo, Japan.

IUPAC Congress

18–22 August
36th IUPAC Congress. Geneva, Switzerland.
Prof. J. Weber, Department of Physical Chemistry, University of Geneva, 30 quai Ernest-Ansermet, 1211 Geneva 4, Switzerland. Tel.: +41 (22) 7026 530 (direct) or +41 (22) 7026 111; Fax: +41 (22) 7026 518; E-mail: weber@sc2a.unige.ch

IUPAC General Assembly

23–30 August
39th IUPAC General Assembly. Geneva, Switzerland.
The IUPAC General Assembly is not open for general participation but restricted to members of IUPAC bodies that meet on this occasion.

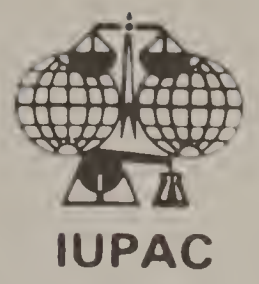
Coordination chemistry

24–29 August
32nd International Conference on Coordination Chemistry. Santiago, Chile.
Prof. J. Costamagna, Departamento de Química, Facultad de Ciencia, Universidad de Santiago di Chile, Casilla 307, Santiago-2, Chile. Tel.: +56 (2) 68 11644; Fax: +56 (2) 68 12108; E-mail: jcostama@lauca.usach.cl

Spectroscopicum internationale

21–26 September
30th Colloquium Spectroscopicum Internationale 1997 (CSI). Melbourne, Australia.
The Meeting Planners, 108 Church Street, Hawthorn Victoria 3122, Australia. Tel.: +61 (3) 981 93700; Fax: +61 (3) 981 95978.

International Union of Pure and Applied Chemistry (IUPAC)



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The International Union of Pure and Applied Chemistry (IUPAC), formed in 1919, is a voluntary non-governmental, non-profit association of organizations, each of which represents the chemists of a member country.

Its objectives are:

- to promote continuing co-operation among the chemists of the member countries;
- to study topics of international importance to pure and applied chemistry which need regulation, standardization, or codification;
- to co-operate with other international organizations which deal with topics of a chemical nature;
- to contribute to the advancement of pure and applied chemistry in all its aspects.

The membership of IUPAC presently comprises 40 countries, each represented by a national organization, such as an academy of science or research council.

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Australian Academy of Science **(Australia)**
Österreichische Akademie der Wissenschaften **(Austria)**
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Association of Greek Chemists **(Greece)**
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Chemistry International

IUPAC

1996, Vol. 18, No. 3 (May)

81 Bohuslav Brauner's contributions to our knowledge of atomic weights
Steffen Peiser and Jaroslav Kahovec

83 Letters to the Editor

86 IUPAC–UNESCO collaboration

91 Trapping single atoms and ions

94 News

99 Recent Reports

104 New publications

116 Conferences

117 Conference Calendar

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Front cover: Geneva—location of the 36th IUPAC Congress, 17–22 August 1997.
Further details may be found in this issue (p.193).

International Union of Pure and Applied Chemistry

Changes at the IUPAC Secretariat

For the last 28 years, the Secretariat of IUPAC has been located in Oxford (UK) and has been run by the Executive Secretary Dr Mo Williams. However, at a recent meeting of the Executive Committee of IUPAC it was decided to move the Secretariat from Oxford to the Research Triangle Park, North Carolina, USA; this move to take place during 1997. Further details about this move, and about the new location of the Secretariat, will be given in the Secretary-General's Column which will appear in the next issue (September 1996) of *Chemistry International.*

This move of the Secretariat coincides with the retirement of Dr Mo Williams in April 1997, after 29 years of sterling service to the Union. Further details about the post of Executive Secretary will be forthcoming on the IUPAC World Wide Web page *(http://chemistry.rsc.org/rsc/iupac.htm).*

Air pollution problems in Korea

Youn Yong Lee

Korea Institute of Science and Technology

As a result of the rapid economic development and industrialization over the last three decades, Korea has emerged from an agricultural economy to a heavily industrialized country. This rapid evolution has caused great changes in the society and life-style of the people. One of the major changes has been the migration of people from rural areas to the cities and to industrial complexes. Once-small villages have become large towns, and towns have grown to cities, their population rises rapidly and may range from several hundred thousands to several millions. Before industrialization, more than 80% of the population lived in rural areas, but now more than 85% of the population of Korea, 45 million, live in the cities and industrial complexes. About 25 million of these live in the metropolitan area of Seoul. Consequently, air pollution problems in the cities and industrial complexes of Korea have now become a serious environmental issue.

Public concern about air pollution in Korea has increased since the mid-1970s when the people began to feel the deterioration of the air quality in the cities and the government started to take actions to tackle the air pollution problems. The government enacted the *Comprehensive Environmental Protection Law* in 1977, and amended it in 1979. However, it was only after the Ministry of Environment was established in 1980 that the government made serious efforts to improve the quality of air in Korea by enacting new laws and enforcing strict policy and control measures. According to new standards of ambient air quality that came into effect in 1995, six air pollutants: SO_2, NO_2, TSP, O_3, CO and Pb, are regulated, and according to emission standards, the production of 26 other substances are regulated.

The major pollutant of air in Korea has been sulphur dioxide that is produced by burning sulphur-rich fossil fuels in factories, households and power plants, from the exhausts of automobiles, and from other sources. In the industrial complexes of Ulsan and Yeochon, an appreciable amount of sulphur dioxide comes from the production of sulphuric acid and fertilizers. The total volume of sulphur dioxide emitted in the air in 1992 was estimated to be 1613 549 metric tons. Of this pollution, 49.7% was emitted from industries, and the rest from the heating (16.9%), transportation (14.5%) and power plants (18.9%).

In order to reduce the level of sulphur dioxide in the air, a series of measures were enacted such as the introduction of low-level sulphur fuels in 1980, the regulation of the use of sulphur-rich fuels in 1984, and the regulation and enforcement of the use of LNG in large cities and industry in 1988. The use of solid fuel was banned in five large cities and the Seoul metropolitan area in 1991.

As a result of these measures, the levels of sulphur

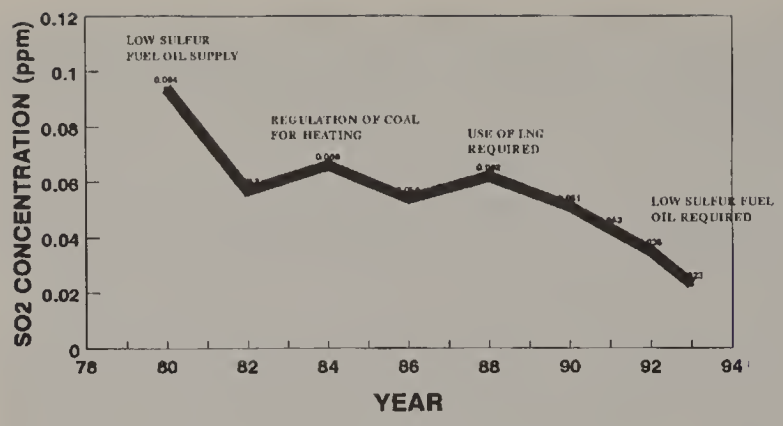

Fig. 1 Annual average concentration of SO_2 in Seoul.

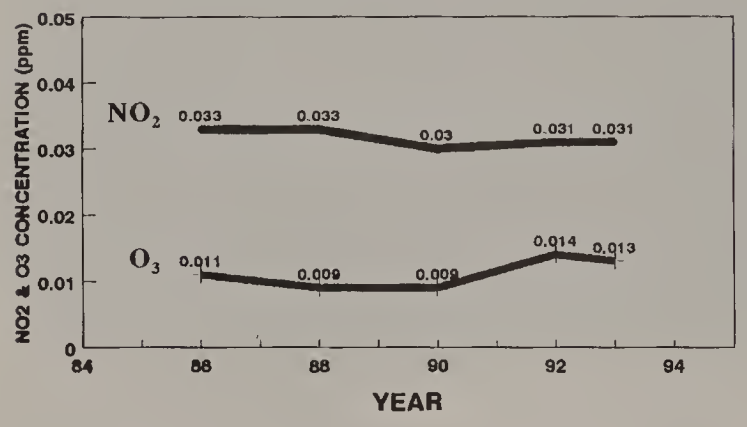

Fig. 2 Variation in the concentrations of NO_2 and O_3 in Seoul.

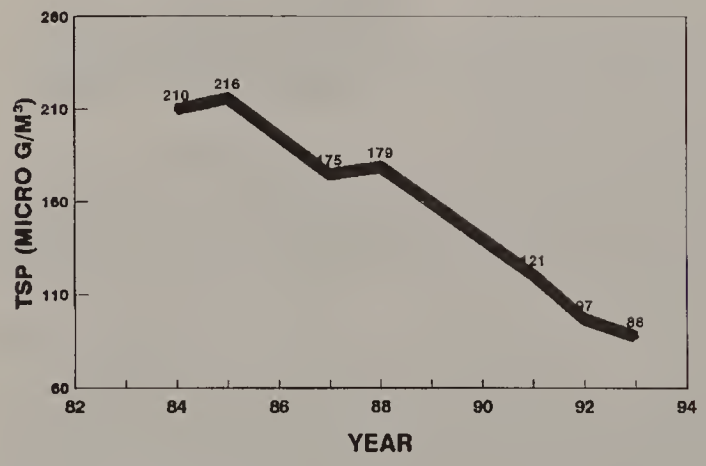

Fig. 3 TSP in Seoul.

dioxide have been reduced in the large cities (Fig. 1). The most dramatic reduction in the level of sulphur dioxide has been witnessed in Seoul. The peak concentration of sulphur dioxide in the air of Seoul recorded in 1980 was 0.094 ppm, but in 1993 it had decreased to 0.023 ppm, i.e. lower than the 0.03 ppm set by the Korean Standard. There are seasonal and regional variations in the level of sulphur dioxide, usually higher in the winter and lower in the summer in the cities, but in the industrial complexes a seasonal variation is not noticeable. In order to further reduce the level of sulphur dioxide in the air, it is necessary to supply these cleaner fuels to wider areas and to lower the sulphur content in the fuel.

Dust pollution in major cities has been steadily declining since the first measurements of dust levels were made in 1984. In Seoul, the dust density was 210 μg/m³ in 1984, but it decreased to 88 μg/m³ in 1993, which is

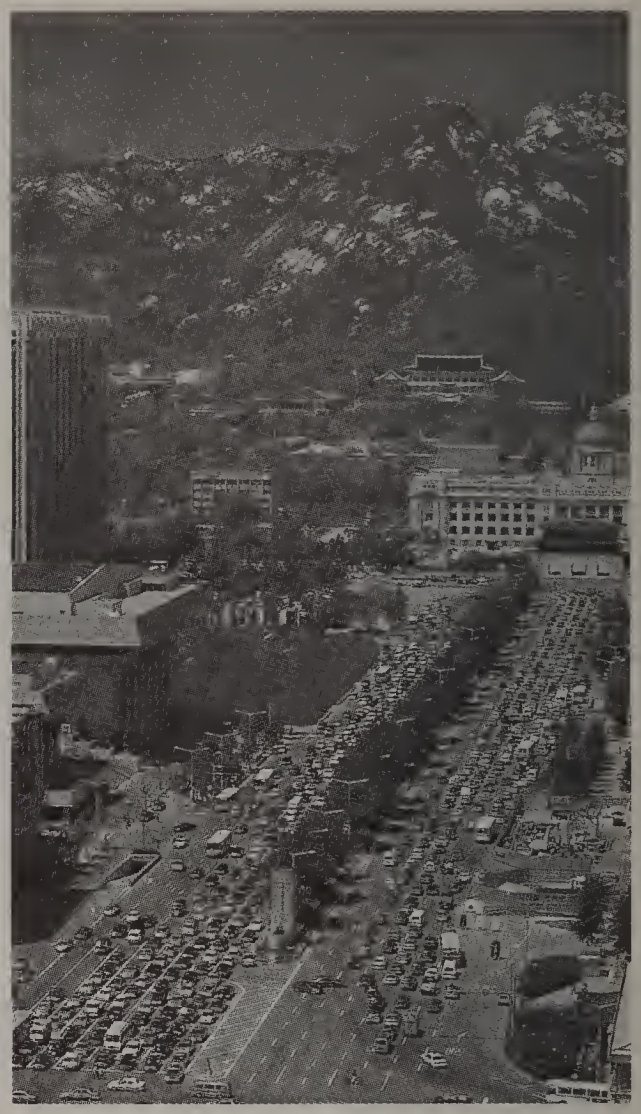

Fig. 4 Clear day in Seoul.

well below the standard level of 150 μg/m³ (Fig. 3). Levels in other large cities in 1993 ranged from 53 to 105 μg/m³. There are seasonal changes in dust pollution. It is at its worst in the spring due to the transboundary movement of yellow sands. Any further reduction in dust pollution in Korea is not expected in the near future as the number of automobiles increases rapidly and the large-scale construction works of subways and apartment buildings continue in the large cities.

The acidity of the rain has been measured in Korea since 1986 at 42 sites in 30 cities. The acidity measured in 1993 and expressed in pH ranges from 5.3 to 5.8, and these values are not very different from those measured in 1986. There are seasonal variations in the acidity of the rain, showing higher acidity in the winter.

Standards for NO_2, O_3, HC and CO were established in 1983 (Fig. 2). There were 84 measurement sites in 35 cities in 1994. Currently, the levels of these contaminants are below the set standards, but as the number of automobiles rapidly increases, it is anticipated that these contaminants will soon become major pollutants in the air, especially in large cities.

As the standard of living rises in Korea, the number of automobiles has increased rapidly in recent years, and it is anticipated that automobile exhaust gases will become the major pollution source in the near future. In 1965, there were only 40 000 automobiles in Korea, but

Fig. 5 Air pollution in Seoul.

the number increased to more than 8 million in 1995. It is expected that the number of automobiles in Korea will reach 13 million by the year 2000. When the total number of automobiles in Korea was 5.2 million in 1992, it was estimated that automobiles emitted 1.84 million tons of pollutants into to the air, accounting for 37.8% of all the air pollution. It was estimated that these automobile exhausts account for 83.3% of HC pollution, 65% of CO, 43% of NO_x, 19.3% TSP and 6.1% of sulphur dioxide. The government has taken series of measures since 1980 in order to reduce automobile exhausts.

The government established strict emission standards for passenger cars with gasoline and LPG-powered engines, emission standards for light oil engine vehicles, and emission standards for all motorcycles. All newly manufactured automobiles in Korea have been required, since 1988, to be equipped with catalytic converter. As a result, in 1993, 93% of all automobiles on the road were equipped with a converter. A manufacturers' warranty system was introduced in 1993 to ensure that car makers guarantee the exhaust systems of their products. The terms of the warranty were strengthened in 1993 to enforce more stringent emission standards. Car manufacturers were allowed to make small buses and trucks with gasoline or LPG-powered engines instead of diesel engines from 1990. The power of engines for big urban commuter buses was planned in 1991 to increase from 185 to 230 horsepower in order to reduce emissions due to overloading. The standards of fuel have been upgraded. Since 1993, lead was removed entirely from any kind of fuel and the use of phosphorous was restricted. Aromatic hydrocarbons, benzene and oxygen are regulated, and the sulphur content has been reduced from 0.20% to 0.15%.

In order to give technical support to national efforts to improve air quality, in 1992 the government launched a national environmental R&D programme called the HAN Project. In accordance with this programme, research on air pollution problems are presently conducted in several research institutes and universities with the financial support of both industry and the government.

As the industrialization of the country continues and the number of automobiles increases, causing heavy traffic congestion in the cities of Korea, it is not expected that air quality will be drastically improved in the short-term. However, as the public awareness of air pollution problems rises with the rising standard of living, and the consensus on economically sustainable development is widened across industry, there will be enhanced efforts by the government and industry to improve the quality of air in Korea.

This short article forms part of a series, submited through the Commission on Atmospheric Chemistry from the Division of Chemistry and the Environment, which highlights local problems of pollution in different countries.

Prague Meetings on Macromolecules

Dr Pavel Čefelín

The Prague Meetings on Macromolecules (PMM) are well known to many of those engaged in research on macromolecules and macromolecular systems. Since monothematic microsymposia and discussion conferences, in the Prague Meetings on Macromolecules series, have been mostly held under the auspices of IUPAC, and have therefore become established as the IUPAC monothematic meetings on macromolecules, it might be of interest to give here something of the history of the Prague Meetings on Macromolecules, and to outline their future programme.

It was after the IUPAC International Symposium on Macromolecules in Prague in 1965 (MACRO 65), when Dr Blahoslav Sedlácek, the then Scientific Secretary of the Institute of Ma̋cromolecular Chemistry of the Czechoslovak Academy of Sciences, Prague, started to implement his vision of an annual Prague Meetings on Macromolecules as a monothematic microsymposium and discussion conference on macromolecules. These meetings were to be sponsored by the newly constituting IUPAC Macromolecular Division.

A meeting was envisaged to consist of plenary sessions only, at which invited main lectures, special communications, and discussion contributions would be presented. Discussion sessions were to be scheduled at discussion conferences. The first Prague Meetings on Macromolecules microsymposium took place in 1967, and the Prague Meetings on Macromolecules soon gained a reputation as meetings with highly specialized topics, careful preparation of scientific and social programmes, and versatile care of the participants. The original conception of the Prague Meetings on Macromolecules has been maintained up to the present time. Dr Sedl Yek, the mastermind of the Prague Meetings on Macromolecules, chaired the Prague Meetings on Macromolecules Organizing Committee until 1972, and acted as the Prague Meetings on Macromolecules Editor afterwards (1973–1989).

Since 1967, thirty-six PMM Microsymposia and sixteen PMM Discussion Conferences have been organized by the Institute of Macromolecular Chemistry in Prague: 1967—1st Microsymposia 'Polymer Gels and Concentrated Solutions'; 1968—2nd Microsymposia 'Structure of Organic Solids', 3rd Microsymposia 'Distribution Analysis and Fractionation of Polymers'; 1969—4th Microsymposia 'Rheology of Polymer Solids and Concentrated Solutions', 5th Microsymposia 'Cyclopolymers and Cyclopolymerization', 6th Microsymposia 'Light Scattering in Polymer Science'; 1970—7th Microsymposia 'Poly(vinyl chloride): Its Formation and Properties', 1st Discussion Conferences 'Models of Biopolymers: Structures and Functions'; 1971—8th Microsymposia 'Morphology of Polymers', 9th Microsymposia 'Thermodynamics of Interactions in Polymer Solutions'; 1972—2nd Discussion Conferences 'Macromolecular Matrices and Carriers of Biological Functions', 10th Microsymposia 'Conformational Structure of Polymers', 11th Microsymposia 'Mechanisms of Inhibition Processes in Polymers: Oxidative and Photochemical Degradation', 3rd Discussion Conferences 'General Principles of Rheology'; 1973—12th Microsymposia 'Organized Structures in Polymer Solutions and Gels', 13th Microsymposia 'Transformation of Functional Groups in Polymers'; 1974—14th Microsymposia 'Crosslinking and Networks', 4th Discussion Conferences' Hetrogeneities in Polymers'; 1975—15th Microsymposia 'Degradation and Stabilization of Polymers'; 1976—5th Discussion Conferences 'Phases and Interfaces in Macromolecular Systems', 16th 'Advances in Scattering Methods'; 1977—17th Microsymposia 'Medical Polymers: Chemical Problems'; 1978—18th Microsymposia 'Synthetic and Semisynthetic Polymer Catalysts and Affinants', 6th Discussion Conferences 'Chromatography of Polymers and Polymers in Chromatography'; 1979—19th Microsymposia 'Mechanisms of Degradation and Stabilization of Hydrocarbon Polymers'. The 20th Microsymposium was entitled 'Microcalorimetry of Macromolecules'; 1980—7th Discussion Conferences 'Polymer Networks', 21st Microsymposia 'Ring-Opening Polymerization of Heterocycles'; 1981—22nd Microsymposia 'Characterization of Structure and Dynamics of Macromolecular Systems by NMR Methods'; 1982—23rd Microsymposia 'Selective Polymeric Sorbents'; 1983—24th Microsymposia 'Copolymers: Structure and Solution Properties', 25th Microsymposia 'Long-Term Stabilities of Hydrocarbon Polymers'; 1984—26th Microsymposia 'Polymers in Medicine and Biology', 27th Microsymposia 'Physical Optics of Dynamic Phenomena and Processes in Macromolecular Systems'; 1985—28th Microsymposia 'Polymer Composites', 8th Discussion Conferences 'Morphology of Polymers'; 1986—29th Microsymposia 'Synthetic Polymer Membranes', 9th Discussion Conferences 'Crosslinked Epoxies'; 1987—30th Microsymposia 'Polymer-Supported Organic Reagents and Catalysts', 10th Discussion Conferences 'Small-Angle Scattering and Related Methods'; 1988—11th Discussion Conferences 'Chemical and Physical Phenomena in Ageing of Polymers', 31st Microsymposia 'Poly(vinyl chloride)'; 1989—12th Discussion Conferences 'Magnetic Resonance in Polymers', 32nd Microsymposia 'Polymer Blends'; 1990—13th Discussion Conferences 'Mechanisms of Polymer Strength and Toughness'; 1991—14th Discussion Conferences 'Rheology of Polymer

Melts'; 1993—33rd Microsymposia 'Optics and Dynamics of Polymers', 34th Microsymposia 'Fluorinated Monomers and Polymers', 15th Discussion Conferences 'Wichterle's Days of Contact Lenses'; 1994—35th Microsymposia 'Polymer Netwoks'; 1995—36th Microsymposia 'High-Swelling Gels', and 16th Discussion Conferences 'Morphology of Polymers'. Periodicity in some evergreen topics is obvious. Since 1967 onwards, the series of PMMs was interrupted only once, in 1992, when the 34th IUPAC International Symposium on Macromolecules took place in Prague.

The following PMM microsymposia and discussion conferences are to be held with sponsorship of the IUPAC Macromolecular Division: 37th Microsymposia '(Bio)Degradable Polymers: Chemical, Biological and Environmental Aspects' (15–16 July, 1996), 38th Microsymposia 'Recycling of Polymers' (14–17 July, 1997), 17th Discussion Conferences 'Surface and Interfacial Phenomena in Macromolecular Systems' (21–24 July, 1997), 18th Discussion Conferences 'Mechanical Behaviour of Polymeric Materials' (20–23 July, 1998), 39th Microsymposia 'Advances in Polymerization Methods: Controlled Synthesis of Functional Polymers' (12–15 July, 1999), 19th Discussion Conferences 'Rheology of Polymer Systems' (19–22 July, 1999), 40th Microsymposia 'Polymers in Medicine' (17–22 July, 2000), 20th Discussion Conferences 'Scattering Methods for the Investigation of Polymers' (9–12 July, 2001), and 41st Microsymposia 'Polymer Membranes' 16–19 July, 2001). The author, Dr Pavel Cefelín, is the PMM Coordinator and an Associate Member, Macromolecular Division Committee of IUPAC.

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Electronic publishing

At the end of last February, a meeting of international experts in all aspects of electronic publishing was organized in Paris by the International Council of Scientific unions (ICSU) and the United Nations' Educational, Scientific and Cultural Organization (UNESCO). This meeting brought together those involved in scientific publishing: scientists (the producers and main end-users of scientific information), publishers, editors and librarians, in an effort to try and obtain a consensus, or even an idea, of what is the current status of the inevitable move from print-on-paper publishing to purely electronic publishing of scientific data.

When one encounters publishers talking about issuing an electronic document, they invariably mean making such a document available on the World Wide Web, for general or restricted access. As, I am sure, with the majority of those who have 'surfed the Web', I have been struck by the bewildering array of information already available to open examination—one can read about anything, from the latest experiments on antimatter at CERN to descriptions of modern witches' covens and rites. However, from what I have seen during my surfing trips I am both continually surprised at the usefulness of some of the material available, but also sometimes taken aback by other things that I have found.

The Web is undoubtedly useful and will certainly change the way science is undertaken and reported. However, the Web contains a lot of rubbish. I recently used a well known search programme to look at chemistry sites, for the most part these gave me access to the information I wanted, however, leading the list of alphabetically displayed subheadings was Alchemy, which proved to contain numerous subsubheadings on topics such as: Alchemy Institute of Healing Arts, and the Book of Quintessence. What the Book of Quintessence is I have no idea, and no interest in finding out, however, the presence of this nonsense amongst more appropriate and useful material is disquieting. We are continually told that the quality of scientific teaching and the general scientific awareness of the population is falling, such a situation is particularly alarming when one sees this free, uncontrolled mixing of science and nonscience/pseudoscience and all easily accessible.

Perhaps it is too late to try and bring order to the Web, that is to better compartmentalize and regulate what is available—which is what conventional publishing on paper achieves. The Internet and its most visible manifestation, the Web, is evolving at a phenomenal rate—experts are now saying that a new generation in the technology comes every 2 years. It is the necessity of getting to grips with this rapid evolution, and at least attempting to bring some order to the current semi-

The UNESCO Headquarters in Paris—site of the recent conference on electronic publishing.

chaos in the dissemination of scientific information that prompted the above mentioned meeting of experts in electronic publishing in Paris.

For almost a week, the Conference of Experts in Electronic Publishing convened by the ICSU and UNESCO discussed the broad range of problems and opportunities presented by the new information technologies. The Conference approved a number of recommendations, roughly grouped under five headings which are directed specifically to ICSU and UNESCO, and through them to the scientific community in general, the learned societies and national academies, and others involved in the provision and archiving of scientific information such as publishers and librarians, and to national governments.

The Conference was divided into plenary lectures and working sessions. In the plenary presentations, experts spoke about: Current Status of Electronic Publishing; Electronic Data Storage, Access and Archiving; Tools and Standards for Protection, Control and Presentation of Data; Legal and Ethical Issues in Electronic Publishing; The Scientists' View of Electronic Publishing; Views of Learned Societies and Professional Scientific Publishers; Economics and Organization of primary Electronic Publishing; and Options for the Future.

Some of the ideas for the future were quite radical. For example, the International Union of Pure and Applied Physics (IUPAP) argued that the traditional path for the publication of scientific information should be abandoned and replaced by a system in which the scientific societies take central stage. Saying that the current problems of ever increasing cost, ever increasing delays and inadequate peer review could be solved without loss of the benefits of electronic publishing. In principle, IUPAP would like to see a full text database, administered by regional physical societies, with links to existing journals for the refereeing, printing and mailing of papers, to be published in both paper and electronic journals, thereby allowing the Physical Societies to take over responsibility for publishing physics.

For half of the Conference, the 150 delegates split up into smaller working groups to address the following issues in some detail. The make-up of the working groups was very much determined by the particular interest or expertise of the individual delegates. Some of the more important and far-reaching recommendations are given here:

Peer-review and codes of practice

There were a number of fundamental questions which this working group—made up of those who had a specific interest in, or experience of, peer-review—sought to address. For example, how will peer review be undertaken for purely electronic journals? Will it differ substantially for electronic-only journals and will there still have to be a parallel, but different, system maintained for print-on-paper journals? This of course, illustrates the biggest question for publishers—how long will publishers continue to print their journals on paper and, at the same time, disseminate an electronic version? Maintaining the two systems together will certainly be more expensive than either approach individually.

Some of these questions were answered by Prof. S. R. Hall, a crystallographer from the University of Western Australia, who explained that the journal *Acta Crystallographica C*, published by the International Union of Crystallography, is now an established peer-reviewed electronic journal. The 'manuscript' is submitted to the *Acta C* office as a machine-readable information package which contains much more information than will eventually be published in the journal, for example, the raw experimental data. This electronic manuscript, called a CIF and prepared using software developed by the International Union of Crystallography, is sent electronically by an editor to an appropriate referee. The referee then views the CIF and responds electronically. If necessary, the CIF then goes back to the author, and his responses and changes are

also made electronically. A final print-on-paper 'hard copy' is made only at the last minute in the production office. Apparently, the system works well and the crystallography community is well versed in the use of electronic means of communications. Summing up the current practice in crystallography journals, Hall said that electronic submission is as important as electronic delivery of the final journal. To take full advantage of modern technology, the whole process from author to library needs to be electronic. Indeed, as he pointed out, it is likely that the reader is the least flexible part of the electronic publishing process.

There has been much talk, and no little fear, that the advent of electronic publishing would do away with peer-review. For example, there are many in the high-energy physics community who use electronic bulletin boards—which are unedited and unrefereed—as the place where a scientist would post his results, and from which they would be disseminated to his colleagues. However, in what many found a surprising decision, the Conference overwhelmingly supported the continued need for, and use of, strict peer-review of material submitted for publication in electronic journals. The Conference recommended that the peer-review process should however, yield definitive authenticated and dated versions of papers for publication, although the subsequent attachment of labels or tags indicating later developments or revisions of papers should not be precluded. Related to this last point, attention should be given to the definition of acceptable methods of establishing priority of publication. Apparently, such criteria for establishing priority differ between disciplines. It was felt that ICSU/UNESCO should be encouraged to convene an assembly of scientific societies to formulate codes of ethics and of conduct for electronic publication which would detail the reciprocal obligations of the scientists and the community on matters such as peer review, citation, integrity and authentication of material and the archiving of such material.

Some notes of caution on this brave new world of electronic scientific publishing were given by Nobel laureate Prof. J. Lederberg (Rockefeller University). Lederberg noted that we should not accept without caution the potential fluidity of an electronic document. Certainly it is useful to have flexibility with digitized files—they are readily amended and changed. However, a point must come when the author is prepared to commit his ideas—previously the moment of publication. When the journal appeared on the library shelf it was too late to change your mind, your ideas and opinions are there for all to see and you must respond to your critics. This point of crystallization of an idea is not so obvious with electronically stored files which are easily edited and easily revised. However, a point of commitment is essential—if nothing else because it sets a date for establishing priority in a discovery or in the evolution of a field of research.

Lederberg's comments raised many questions about how the integrity of the data stored in an electronic archive could be guaranteed. Once a set of data had been authenticated, that is, when a manuscript has been revised sufficiently and the author is prepared, at that time, to call his work definitive, and the data were finally deposited in an archive, how could we ensure that this dataset was not going to be 'hacked into' and changed? Indeed, how are the entries in such an archive to be dated? One useful suggestion to allow one to distinguish between a refereed and unrefereed archived document would be to place a mark (a circle with the letter R inscribed within it was suggested) on the document which had been 'approved' by some expert person/group—others suggested that the logo of a recognized learned society could be appended to the file and used for this purpose.

The electronic archive

Given that traditional print-on-paper publication automatically creates an archive, it was considered timely and urgent that attention be given to ensuring the archiving of science in electronic formats. Everyone agreed that a permanent record of scientific achievement was essential, but who would create this archive and who would maintain and pay for it?

The ease of access to, and the malleable nature of, digitised information requires the creation of verifiable electronic archives which would include databases. It was recommended that scientific societies, publishers and librarians come together to establish guidelines for such electronic archives. These guidelines should include, but not be limited to: maintenance, content, structure (including metadata—the peripheral data which define the format of the main data in the archive), finance, eligibility, accessibility and interpretability. As it is likely that many electronic archives will eventually be established, the Conference recommended that a registry of electronic archives in scientific fields be established—including guidelines and principles of operation. Many of these points relate directly to the need to establish international standards in telecommunications and data storage which have importance well away from the world of scientific research.

Financial considerations

The Conference recommended that funding agencies should regard as an essential part of scientific research funding the costs both of publishing results and of information provision. The Conference recognized that the provision of electronic information in a searchable form is potentially of considerable importance to the scientific community for the efficient conduct of research and

education. Funds should be directed to allow use to be made of the full potential and development of this source of information.

Many publishers stated that if the costs of paper, printing, binding and distribution are removed then there are significant savings to be made in scientific publishing. However, such estimates of the savings varied dramatically because the costs of electronic publishing varied so widely between countries and amongst publishers. Indeed, it was deemed necessary to recommend that a study of the costs and benefits of electronic publishing should be carried out by the ICSU in coordination with its member organizations and organizations representing the information and publishing community.

Many suggested that page charges be reintroduced to cover the costs of archiving of documents and to replace copyright charges. Indeed, Prof. Lederberg commented that page charges would be an ideal means of controlling those authors who, in the absence of strong editors and competent peer-reviewers, will write longer and longer articles, because there is, in principle, no limit on how long an electronic manuscript in an electronic journal could become.

Training and work-styles

Although each scientific discipline has its own particular method of information acquisition and dissemination, a set of basic skills needed by scientists can nevertheless be identified. It was recommended that all scientists should receive training in information resources and library use, and in how to write well, particularly with regard to the electronic medium. Such skills should be acquired as early as possible in their career. ICSU and UNESCO should assist those developing countries which do not have the resources and expertise to organize such training.

It was recognised that an adequate and reasonably priced network access is essential for scientific work and education today. National authorities should ensure that the appropriate infrastructure is established for this purpose and that scientific data traffic receives appropriate priority. Scientists in developing countries should have access to computer communications to participate in information exchange with colleagues in industrialized countries, and ICSU and UNESCO should promote such access with available means.

In keeping with the increasing role of the scientist in the process of electronic publishing, the international scientific community should facilitate the exchange of experience between scientists in different disciplines, with a view to identifying best practice and encouraging cooperative training, research and development. As a useful first step, an information network should be established to refer users to information resources, tools and standards relating to electronic publishing in science. Direct, immediate access to this information should be incorporated into the ICSU World Wide Web site (http://www.lmcp.jussieu.fr/icsu/) and facilities should be provided via e-mail for those users without WWW capacity.

Developing countries

The scientific community in developing countries will, it was hoped, become involved in all stages of electronic publishing, including locally published on-line journals, CD-ROM technology and appropriate databases. They should assume greater control of the technologies involved. UNESCO, ICSU and the international community should take this into account in planning and implementing cooperative projects. The scientific community in developing countries should become involved as partners in the development of standards, archiving and library services so that these may be better adapted to their local needs. In particular, regional cooperation should be encouraged and language-independent systems adopted where possible. UNESCO should encourage support for one or two pilot projects in electronic publishing in the developing world.

Finally, it was noted that the costs of infrastructure and information provision in developing countries are particularly high, and that UNESCO and other United Nations' Agencies should become involved in promoting and encouraging deregulation and competition within developing countries as a means of reducing the current high costs.

General

Many of these recommendations are of considerable practical importance and could be implemented without much delay or new finance. However, it was recognized by the Conference that some of the recommendations would require considerable new financial support from national governments which is not likely to be forthcoming in the near, or indeed long-term, future. In particular, the recommendation that national governments ensure that scientists have privileged and cheap access to electronic communications goes counter to the very great drive currently being observed in the industrialized world for a deregulated telecommunications market. In the developed world, it is the market which will decided what is the cost of telecommunications, prices have been falling continually with increased international competition. It is likely that scientists are going to have to work within this framework and cannot expect special treatment.

The Conference also identified a shift towards the use of raw scientific data (e.g. audio recordings and video images in publications) and a lack of a common

standard for the handling of such material—at present there are at least six incompatible protocols being used for rotating molecules and other such figures in electronic documents. The meeting stopped short of calling for a common standard, but it did insist that some guidelines be established—it may become inevitable that standards from the multimedia industry be adopted by those producing scientific electronic publications.

Throughout the Conference there was much criticism of professional publishers. A UK-based consultant, Douglas Armati, pointed out that publishers insist on holding onto the dogma of a 'dying transaction paradigm' in their electronic publishing ventures based on a system of subscription that has 'served them well and profitably.' Many scientists commented that they resented the large profits made by many publishers from their academic journals business.

Publishers have until now defined their operations in terms of the mechanism of distribution and production. Armati argued that electronic publishing changes the traditional academic publishing model of obtaining content, largely without cost, and selling back to the contributor base (the scientists) at high prices. But many commercial publishers and learned societies contested such arguments about the new electronic medium of publishing being much cheaper than publication on paper. They point out that major cost savings would entail researchers taking on much of the work now undertaken by publishers. Previously, scientists had been able to get on with their research, now they will have to become more closely involved in the preparation and formatting of their work. Similarly, a representative of a large commercial publisher pointed out that the predicted increase in the amount of raw data to be archived electronically would mean that publishers would increasingly have to take responsibility for validating such data, and that this would certainly bring new costs. Such arguments led to discussions about who should set-up and run the archiving system of the future.

All of these bewildering changes give one unsettling intimations about the future of scientific publishing. One gained an impression in the plenary sessions of this meeting that everybody present knew they should be doing something with the new technology to create a new world of electronic journals, books, etc. However, the technology is evolving rapidly and the people who have been involved in publishing for some time are not the most expert in computer technology, the result being that there was no consensus as to what should be done, let alone how it should be acheived.

However, things are changing. Previously, an author when his own manuscript had finally been accepted could relax; sitting in the library in a comfortable deep armchair browsing through a pile of promising journals in search of something interesting and perhaps entertaining to pass an odd hour. In the future, however, as some of the more enthusiastic physicists involved in electronic publishing pointed out, 'the journal will be a set of linked Web resources' which will give the user an 'access point to the data continuum', and 'electronic journals are now not isolated in space and time, they can become the whole Internet with links to numerous other disciplines.' Which certainly implies that even casual readers will have to be prepared to make substantial adaptations in future.

Report of the International Union of Pure and Applied Chemistry

Mo Williams
Executive Secretary

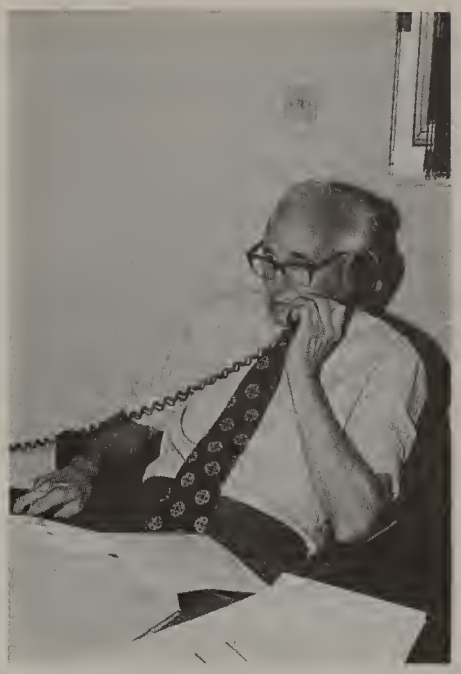
The main event for IUPAC in 1995 was its 38th General Assembly (GA), which was held during August at University of Surrey, Guildford, UK. Delegates from 39 of the 41 National Adhering Organizations (NAOs) were in attendance. Accounts of the deliberations are given in *Chemistry International* (No. 6, 1995; no. 3, 1996).

The IUPAC Officers for the period 1996–1997 are:

President	Prof. A. E. Fischli (Switzerland)
Vice-President	Prof. J. Jortner (Israel)
Past-President	Prof. K. I. Zamaraev (Russia)
Secretary General	Dr E. D. Becker (USA)
Treasurer	Prof. J. M. Ward (UK)

The Members of the Union remained unchanged at 41 NAOs. Bulgaria rejoined IUPAC as an Observer Country, making a total of 16 with such status. There were 31 Associated Organizations.

The ability of the long-standing IUPAC structure of Divisions and Commissions to cope adequately with the complicated scientific problems now faced by society, was improved by restructuring the Applied Chemistry Division and the Clinical Chemistry Division/ Medicinal Chemistry Section as Divisions on *Chemistry and the Environment* and *Chemistry and Human Health*, respectively. The interdisciplinary nature of many problems was also recognized by the creation of a new Commission on Biophysical Chemistry. Further



Dr Mo Williams

major Divisional changes are still under consideration. The implications for IUPAC of the current revolution in scientific communication became the responsibility of a new *Committee on Printed and Electronic Publications*, formed by merging the former Publications and Chemical Databases Committees.

Future scientific directions for the Union and the development of a strategic plan are receiving priority attention from the higher authorities of IUPAC, with a view to discussion with scientific leaders, both inside and outside IUPAC. Whilst the traditional core activities of establishing and codifying the language of chemistry (nomenclature, symbols, units and terminology), the standardization of procedures and materials, and the compilation of critically evaluated data are expected to remain, emphasis will be placed on globally important issues involving chemistry and educating young people world-wide to its concepts and value. Meanwhile, all IUPAC scientific bodies were pressed to review their project programmes with respect to low priority, long time taken for completion, and even justification for being undertaken by an international scientific union.

The first biennium of operation (1994–95) was completed of the pool of titular member positions, which was specially designated in 1993 to carry out work in high-priority areas within a limited period of time (usually 2 years). A start was made at the GA on some major projects approved for 1996–97, including: alternative scenarios for future energy production, and oil spill clean-up and remediation. In addition, in a move to bring more democracy to IUPAC, the Associate Members of all its scientific bodies were granted full voting rights.

Another important subject was the future of the Affiliate Membership Programme (AMP). Because of the decreasing numbers of Affiliates in recent years, the viability for continuation of the Programme was raised at the Council meeting in Guildford. A small group from the Bureau was charged with investigating the possibility of continuing AMP, perhaps in a different form and under a different name. This investigation will automatically involve future policy with respect to the Union's news magazine *Chemistry International*.

The strong criticism provoked from some parts of the world in response to the 1994 IUPAC recommendations on names and symbols for the transfermium elements was reviewed by the Bureau. It voted to reconsider its earlier decision, by adopting the 1994 recommendations as provisional, in full accordance with statutory procedures. Public comment would be invited during January–May 1996, with a view to consideration of submissions in mid-1996 by the Commission on Nomenclature of Inorganic Chemistry (CNIC). It was hoped to reach a final agreement on the recommendations at the 1997 General Assembly. A consensus on the issues, reached at Guildford in a meeting of representatives of the NAOs of Germany, Russia, and USA, was sent to the CNIC.

Significant amongst several important IUPAC publications during 1995 was a report on *Some Problems in the Destruction of Chemical Munitions, and Recommendations towards Their Amelioration*, by the Union's Task Force on Scientific Aspects of the Destruction of Chemical Warfare Agents. The *Compendium of Terminology and Nomenclature of Properties in Clinical Laboratory Sciences*, issued jointly with the International Federation of Clinical Chemistry, was expected to attract wide attention in relevant health areas. The monographs on *Chemistry for the 21st Century* continued its high quality output with the appearance of *Ultrafast Processes in Chemistry and Photobiology*.

Much concern was expressed at the GA about the need for improved publicity, to the chemical community world-wide, for the large amount of outstanding work carried out by the scientific bodies of the Union. This will be remedied to some extent in early 1996, when IUPAC goes on-line with its Home Page on the Internet at: http://chemistry.rsc.org/rsc/iupac.htm

Three projects from IUPAC bodies were supported by ICSU during 1995. A Working Party was able to meet, and to finalize a substantial *Glossary of Terms in*

Fig. 1 Members of the CHEMRAWN Committee at work during the Guildford General Assembly.

Fig. 2 Participants of the Guildford General Assembly relaxing after their hard work during an unusually hot English summer.

Bioinorganic Chemistry for public review, prior to publication in the Union's journal *Pure and Applied Chemistry*. The second project was entitled *Reliability of Analytical Data in Trace Analysis*. Firstly, chemists from the Inorganic Division of IUPAC were able to carry out the sixth round—trace elements in (synthetic and natural) water—in an International Measurement Evaluation Programme, concerned with establishing reliable, traceable and comparable chemical data in important areas such as health, environment and control of waste and chemical processes. In addition, a Working Group from the Analytical Division was able to organize the 6th International Symposium on Harmonization of the Role of Laboratory Quality Assurance in Relation to Total Quality Management (Melbourne, December 1995).

The third project supported by ICSU was on *Processing of Hazardous Waste*, with contributions from three expert groups in different branches of chemistry towards tackling this important and difficult problem. A Task Force from the Physical Division organized a workshop at the 12th International Symposium on Plasma Chemistry (Minneapolis, August 1995), at which overviews were provided of the availability and reliability of thermodynamic and kinetic data for a hazardous substances database. Chemists from the Analytical Division were evaluating the impact of environmental factors on the physical and chemical characterization of small particles in the atmosphere, leading to the publication of a volume in the series *Analytical and Physical Chemistry of Environmental Systems*. Finally, a Working Party was preparing a report, designed to present an unbiased view on the current state-of-the-art of recycling of polymers, for discussion at the 38th Microsymposium on Macromolecules (Prague, 1997).

APPENDIX

The following nomenclature reports (IUPAC Recommendations 1995) were published during the year:

1 Commission on High Temperature and Solid State Chemistry. Recommended terminology for the description of carbon as a solid. *Pure Appl. Chem.* 1995, **67**, 473–506.

2 Commission on Molecular Structure and Spectroscopy. Guidelines on nuclear magnetic resonance computerized databases. *Pure Appl. Chem.* 1995, **67**, 593–596.

3 Commissions on Nomenclature of Organic Chemistry and on Physical Organic Chemistry. Glossary of class names of organic compounds and reactivity intermediates based on structure. *Pure Appl. Chem.* 1995, **67**, 1307–1376.

4 Commission on Atmospheric Chemistry. Units for use in atmospheric chemistry. *Pure Appl. Chem.* 1995, **67**, 1377–1406.

5 Commission on Quantities and Units in Clinical Chemistry. Properties and units in the clinical laboratory sciences—I. Syntax and semantic rules. *Pure Appl. Chem.* 1995, **67**, 1563–1574.

6 Commission on Analytical Nomenclature. Nomenclature in evaluation of analytical methods including detection and quantification capabilities. *Pure Appl. Chem.* 1995, **67**, 1699–1723.

7 Commission on Spectrochemical and Other Optical Procedures for Analysis. Nomenclature, symbols, units and their usage in spectrochemical analysis—IX. Instrumentation for the spectral dispersion and isolation of optical radiation. *Pure Appl. Chem.* 1995, **67**, 1725–1744.

8 Commission on Spectrochemical and Other Optical Procedures for Analysis. Nomenclature, symbols, units and their usage in spectrochemical analysis—XI. Detection of radiation. *Pure Appl. Chem.* 1995, **67**, 1745–1760.

9 Commission on Spectrochemical and Other Optical Procedures for Analysis. Nomenclature, symbols, units and their usage in spectrochemical analysis: Cumulative index of terms: Parts I–XIII. *Pure Appl. Chem.* 1995, **67,** 1761–1779.

10 Commission on Spectrochemical and Other Optical Procedures for Analysis. Nomenclature, symbols, units, and their usage in spectrochemical analysis—XV. Laser-based molecular spectroscopy for chemical analysis: Laser fundamentals. *Pure Appl. Chem.* 1995, **67,** 1913–1928.

11 Joint IUPAC–IFCC Working Party on the Compendium of Terminology and Nomenclature in Clinical Chemistry. *Compendium of Terminology and Nomenclature of Properties in Clinical Laboratory Sciences* (the Silver Book), Oxford, UK: Blackwell Science, 1995.

12 *A Multilingual Glossary of Biotechnological Terms.* Basel, Switerland: VHCA Publishers, 1995.

The following technical reports by IUPAC bodies were published during the year:

1 Interdivisional Working Party on Harmonization of Quality Assurance Schemes for Analytical Laborato-

ries. Protocol for the design, conduct and interpretation of method-performance studies: Revised 1994. *Pure Appl. Chem.* 1995, **67**, 331–344.
2. Commission on Biotechnology. Interrelations of chemistry and biotechnology—V. Biocatalysis on nonconventional media: Medium engineering aspects. *Pure Appl. Chem.* 1995, **67**, 345–373.
3 Commission on Electroanalytical Chemistry. Selectivity coefficients for ion-selective electrodes: Recommended methods for reporting $K^{pot A,B}$ values. *Pure Appl. Chem.* 1995, **67,** 507–518.
4 Commission on General Aspects of Analytical Chemistry. Classification and chemical characteristics of immobilized enzymes. *Pure Appl. Chem.* 1995, **67**, 597–600.
5 Commission on General Aspects of Analytical Chemistry. Catalytic methods of analysis: Characterization, classification and methodology. *Pure Appl. Chem.* 1995, **67**, 601–614.
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11 Commission on Colloid and Surface Chemistry including Catalysis. Manual of methods and procedures for catalyst characterization. *Pure Appl. Chem.* 1995, **67**, 1257–1306.
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13 Commission on Agrochemicals. Detection and significance of active metabolites of agrochemicals and related xenobiotics in animals. *Pure Appl. Chem.* 1995, **67**, 1487–1532.
14 Commission on Water Chemistry. Use of immunoassays for the analysis of pesticides and some other organics in water samples. *Pure Appl. Chem.* 1995, **67**, 1533–1548.
15 Commission on Water Chemistry. In-situ and on-site treatment of groundwater. *Pure Appl. Chem.* 1995, **67**, 1549–1562.
16 Commission on Toxicology. Sample collection guidelines for trace elements in blood and urine. *Pure Appl. Chem.* 1995, **67**, 1575–1608.
17 Commission on Oils, Fats, and Derivatives. Determination of chlorophyll pigments in crude vegetable oils: Results of a collaborative study and the standardized method. *Pure Appl. Chem.* 1995, **67**, 1781–1787.
18 Commission on High Temperature and Solid State Chemistry. The electrical conductivity of cubic stabilized zirconia: Results of an IUPAC collaborative study. *Pure Appl. Chem.* 1995, **67**, 1891–1904.
19 Commission on General Aspects of Analytical Chemistry. Absolute methods in analytical chemistry. *Pure Appl. Chem.* 1995, **67**, 1905–1911.
20 Commission on Radiochemistry and Nuclear Techniques. Isotopic and nuclear analytical techniques in biological systems: A critical study—IX. Neutron activation analysis. *Pure Appl. Chem.* 1995, **67**, 1929–1941.
21 Commission on Radiochemistry and Nuclear Techniques. Isotopic and nuclear analytical techniques in biological systems: A critical study—X. Elemental isotope dilution and analysis with radioactive and stable isotopes. *Pure Appl. Chem.* 1995, **67**, 1943–1949.
22 Commission on Polymer Characterization and Properties. Properties of EDAM copolymers as polypropylene resin modifier. *Pure Appl. Chem.* 1995, **67**, 2047–2056.
23 Commission on Atmospheric Chemistry. Major concerns and research needs for our understanding of the chemistry of the atmosphere. *Pure Appl. Chem.* 1995, **67**, 2057–2064.
24 Commission on Agrochemicals. Immunoassays for residue analysis of agrochemicals: Proposed guidelines for precision, standardization and quality control. *Pure Appl. Chem.* 1995, **67**, 2065–2088.
25 Commission on Agrochemicals. Pesticide runoff: Methods and interpretation of field studies. *Pure Appl. Chem.* 1995, **67**, 2089–2108.
26 Commission on Agrochemicals. Offsite transport of pesticides in water: Mathematical models of pesticide leaching and runoff. *Pure Appl. Chem.* 1995, **67**, 2109–2148.
27 Commission on Molecular Structure and Spectroscopy. *Tables of Intensities for the Calibration of Infrared Spectroscopic Measurements in the Liquid Phase*. Oxford, UK: Blackwell Science, 1995.
28 Chemistry for the 21st Century Monograph—*Ultrafast Processes in Chemistry and Photobiology*. Oxford, UK: Blackwell Science, 1995.
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30 Commission on Solubility Data. Solubility Data Series—Vol. 58. *Polycyclic Aromatic Hydrocarbons: Binary Non-aqueous Systems—Solutes A–E*. Oxford, UK: Oxford University Press, 1995.
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Binary Non-aqueous Systems—Solutes F–Z. Oxford, UK: Oxford University Press, 1995.

32 Commission on Solubility Data. Solubility Data Series—Vol. 60. *Halogenated Methanes with Water* Oxford, UK: Oxford University Press, 1995.

33 Commission on Solubility Data. Solubility Data Series—Vol. 61. *Alkali Metal and Ammonium Perchlorates. Part I. Lithium and Sodium Perchlorates* Oxford, UK: Oxford University Press, 1995.

Twenty-six symposia were sponsored by IUPAC in 1995, namely:

1 2–7 July 1995. 20th International Symposium on Macrocyclic Chemistry, Jerusalem, Israel. [Lectures to be published in *Pure Appl. Chem.*, 1996]

2 5–7 July 1995. International Symposium on Polymer Morphology and Electrical Properties. Lodz, Poland. [Proceedings to be published as a *Macromolecular Symposia* volume by Hüthig & Wepf Verlag, Basel, 1996]

3 9–15 July 1995. SAC 95: International Conference on Analytical Chemistry. Hull, UK. [Published in *The Analyst* 1996, 121 (No. 2)].

4 10–13 July 1995. 5th COMTOX Symposium on Toxicology and Clinical Chemistry of Metals, Vancouver, Canada. [Proceedings to be published in *Annals of Clinical and Laboratory Science,* 1996].

5 16–21 July 1995. 3rd International Symposium on Functional Dyes, Santa Cruz, California, USA. [Lectures to be published in *Pure Appl. Chem.,* 1996]

6 31 July—4 August 1995. 6th International Conference on Chemistry in Africa. [Proceedings to be published by the organizers].

7 31 July—4 August 1995. 8th International Symposium on Novel Aromatic Compounds, Braunschweig, Germany. [*Pure Appl. Chem.* 1996, **68** (2)]

8 30 July—4 August 1995. 4th International Conference on Heteroatom Chemistry, Seoul, Korea. [*Pure Appl. Chem.* 1996, **68** (4)]

9 6–10 August 1995. 8th IUPAC Symposium on Organometallic Chemistry Directed Toward Organic Synthesis. Santa Barbara, California, USA. [*Pure Appl. Chem.* 1996, **68** (1)]

10 6–11 August 1995. 15th International Congress of Heterocyclic Chemistry. Taipei, Taiwan. [Proceedings to be published in *J. Heterocyclic Chemistry*, 1996]

11 14–19 August 1995. 35th IUPAC Congress. Istanbul, Turkey. [Lectures to be published in *Pure Appl. Chem.*, 1996]

12 21–26 August 1995. 12th International Symposium on Plasma Chemistry. Minneapolis, MN, USA. [*Pure Appl. Chem.* 1996, **68** (5)]

13 17 August—1 September 1995. 9th International Conference on Liquid and Amorphous Metals. Chicago (USA) [Proceedings to be published by North-Holland/Elsevier, Amsterdam, 1996]

14 27 August—1 September 1995. 29th Colloquium Spectroscopicum Internationale, Leipzig, Germany. [Proceedings to be published in *Fresenius J. Analyt. Chem.*, 1996]

15 28 August—2 September 1995. International Symposium on Industry—Education Initiatives in Chemistry. [Proceedings to be published by the organizers]

16 29 August—3 September 1995. 24th International Conference on Solution Chemistry. Lisbon, Portugal. [Lectures to be published in *Pure Appl. Chem.*, 1996]

17 3–8 September 1995. AFMC International Medicinal Chemistry Symposium, Tokyo, Japan. [Proceedings to be published by Blackwell Science, Oxford, 1996]

18 4–8 September 1995. International Symposium on Ionic Polymerization, Istanbul, Turkey. [Proceedings to be published as a *Macromolecular Symposia* volume by Hüthig & Wepf Verlag, Basel, 1996]

19 10–16 September 1995. International Conference on the Applications of the Mössbauer Effect, Rimini, Italy. [Proceedings to be published in *Hyperfine Interactions*, 1996]

20 17–23 September 1995. 3rd International Symposium on Bioorganic Chemistry, Dagomys, Sochi, Russia. [Lectures to be published in *Pure Appl. Chem.*, 1996]

21 18–22 September 1995. International Symposium on Chromatography of Polymers and Related Substances. Bratislava, Slovakia. [Proceedings to be published as a *Macromolecular Symposia* volume by Hüthig & Wepf Verlag, Basel, 1996]

22 17–20 October 1995. International Symposium on the Assessment of Respiratory Carcinogenic Risk from Occupational Exposure to Inorganic Substances, Luxembourg. [Proceedings to be published by the organizers, 1996]

23 25–27 October 1995. 2nd International Forum on Environmental Catalysis. Tokyo, Japan. [*Pure Appl. Chem.* 1996, **68** (2)]

24 28 October, 1995. Workshop on Soil Chemistry and Ecosystem Health. St. Louis, MO, USA. [Proceedings to be published by Soil Science Society of America]

25 2–4 November 1995. 6th International Congress on Automation and New Technology in Clinical Laboratory. Sitges, Barcelona, Spain. [Lectures to be published in *Pure Appl. Chem.*]

26 3–6 November 1995. 6th International Symposium on Macromolecule-Metal Complexes, Guangzhou, China. [Proceedings to be published as a *Macromolecular Symposia* volume by Hüthig & Wepf Verlag, Basel, 1996]

IUPAC colleagues deceased

USA: Prof. A. O. Nier (16 May 1994) Commission on Atomic Weights (1947–1963).

UK: Dr. A. A. Smales (15 February 1996) Analytical Chemistry Division Committee (1957–1961, 1963–1967), Commission on Analytical Radiochemistry and Nuclear Materials (1965–1977), Commission on Atomic Weights (1971–1973).

IUPAC Accounts for 1995

Treasurer's comments

At the Council Meeting in Guildford last September I forecast that we should finish the year with a small surplus. In fact, you will see from the accounts that the surplus was a substantial one—USD 113 344. This surplus, added to the 1994 surplus of USD 148 718, gives a 1994–95 biennial surplus of USD 262 062, a further confirmation that the Union's finances are now well under control. We should not however conclude that we will now continue to make substantial surpluses and that we can rely on their potential to increase our expenditure to any marked extent.

Although the 1995 outcome was USD 293.9k better than budget, by far the biggest contribution to it was an underspend of USD 160.6k on the Guildford Assembly, mainly brought about because only 85% of TMs attended and because the cost of air travel remained flat. The 1997 Assembly will be held in Geneva and the 1999 Assembly in Berlin, in both of which expensive city accommodation will need to be in hotels and will consequently cost substantially more than the student accommodation used in Guildford. It is already clear that it will be difficult to keep the total cost of the Geneva Assembly to the budget figure of USD 500k. The next biggest contribution was an underspend of USD 61.7k of the USD 76.1k carried over for IUPAC Bodies (Divisions and Standing Committees) from 1994 as a provision. Other contributions were an underspend of USD 35.9k (12% of budget) by the Secretariat, USD 21.7 over budget from the payment of subscriptions owing from previous years and another good performance by Publications that produced an income USD 15.7k better than budget.

If the Guildford Assembly had cost USD 490k as budgeted, and IUPAC Bodies had spent the whole of their allocation, both of which eventualities might have been expected in a more normal year, 1995 would have shown a deficit of USD 119k (budget deficit was USD 180k), and the result for the biennium a modest, but nevertheless encouraging, surplus of USD 30k. The message to be taken from the 1995 and 1994–95 results is that we have made a useful addition to our reserves, some of which might be used for special short-term initiatives or for extra meetings that might be needed to implement the changes and measures being contemplated to increase our efficiency and visibility. Other uses are discussed further on.

As a result of moving our banking and investments at the end of 1994 from the Union Bank of Switzerland to Merrill Lynch, we started 1995 with about half our investment portfolio in money funds. Most of these funds have now been transferred to mutual equity funds. As these transfers were spread across the year it is difficult to make a precise estimate of the total percentage gain over the year, but taking the 1 January value of the bonds held throughout the year, plus the cost prices of the mutual funds as a basis, the total gain by these holdings was 11%. The total market value of our holdings with Merrill Lynchm, which includes a cash management account used for our day-to-day business and which earns significant interest, grew from USD 2.252m to USD 2.431m during the year, an increase of 7.9%. If to this is added the interest and dividends earned, the result is a total gain of 12.7%. It is appropriate to mention here that in conformity with the latest accountancy practice the securities in the 1995 balance sheet are expressed in terms of market values rather than book or cost values as in previous years.

The Building Fund has been held since its inception in Union Bank of Switzerland GBP funds. When these were sold on transfer of funds to Merrill Lynch it was left to the latter to invest in equities and bonds in whichever currency, GBP or USD, was appropriate. They hesitated over the question for several months and this hesitation and other unfortunate lapses delayed the final investment, still in British funds, until mid-August. The result was a disappointing total gain over the year of 4.7%. Merrill Lynch have apologized for the delay

Auditor's Report

The following is the Report of the Auditors to the IUPAC Executive Committee:

As auditors of the International Union of Pure and Applied Chemistry we have examined the books of account and accounts for the year ended 31 December 1995. Our audit was conducted in accordance with auditing standards promulgated by the profession. We confirm that we meet the legal requirements concerning professional qualification and independence.

Based on our examination, we conclude that the books of account and the accounts are in accordance with Swiss law and the requirements of the statutes.

We recommend that the accounts submitted to you be approved.

NEUTRA TREUHAND AC
Zurich, 20th May, 1994

and there is unlikely to be a repetition; their service is usually very good. At the Finance Committee meeting in February 1996 it was decided to add the equivalent of USD 100 000 from the 1995 surplus to this fund.

It was also agreed to put USD 50 000 into the new sinking fund for an Assembly in the Southern Hemisphere, as was proposed in my report to the 1995 Council Meeting.

IUPAC Accounts 1995 (All amounts expressed in USD)

Comparative Balance Sheet[1]

Liabilities	1995	1994
Capital Account	2513 028	2389 803
Accounts Payable[2]	34 632	23 654
Paulo Franzosini Fund	5659	5659
Provisions & Subaccounts[3]	87 376	190 914
Prepaid Subscriptions[4]	3900	20 650
Sundry Creditors	6635	10 959
Capital Gains Realized[5]	–17 919	–25 493
Unrealized Profit on Securities[8]	89 381	–
Excess of Income over Expenses	113 344	148 718
USD	2836 036	2764 864

Assets	1995	1994
Fixed Assets[6]	22 502	37 345
Cash in Banks[7]	407 228	865 287
Marketable Securities[8]	2043 746	1500 642
Building Fund (held in GBP)[9]	302 942	288 724
Accounts Receivable[10]	23 368	10 029
Subscriptions, etc., Outstanding[11]	36 250	62 837
USD	2836 036	2764 864

Summary of Income and Expenses

	1995	1994
General Expenses net	–40 849	–16 211
Publications Income net	155 732	164 929
Affiliate Membership Programme Expenses net	–1539	0
To Capital Account USD	113 344	148 718

General Income and Expenses

Income	1995	1994
National Subscriptions[12]	630 712	599 762
Company Associate Service Charges[13]	9000	9350
Observer Country Service Charges[14]	1100	650

Finance Committee meeting in Zurich; left to right, Dr J. Brunner, Prof. E.J. Grzywa, Prof. John Ward (IUPAC Treasurer and Chairman) and Dr E.P. Przybylowicz, with Dr Mo Williams (Secretary) standing.

Associated Organization Service Charges[15]	1550	1650
Interest & Dividends Earned	107 854	108 207
Debit to Capital Account	40 849	16 211
USD	791 065	735 830

Expenses	1995	1994
Office Expenses[16]	290 907	312 305
Expenses IUPAC Bodies:		
Standing Committees	35 384	76 562
Divisions[17]	108 956	151 866
General Assembly	329 411	7901
Bad Debts Write Off[18]	–44	44
Bad Debts Provision	–10 888	–44
Other Expenses	88 899	74 283[19]
Foreign Exchange Differences	5726	19 049
Depreciation	18 786	17 792
Provisions: Committed Expenses	–76 072	76 072
USD	791 065	735 830

Publications Income and Expenses

Income	1995	1994
Publications: Blackwell	331 682	323 221
Publications: Pergamon	0	732
Publications: Other Publishers	13 922	16 732
Publications: Secretariat	218	147
BS Support of Publication Activities	20 000	20 000
Miscellaneous Income	0	577
USD	365 822	361 409

Expenses	1995	1994
IUPAC Secretariat (Pubns.)	179 965	170 388
Chem. Intl. to Symposia	351	557
Miscellaneous Expenses[20]	29 774	25 535
Credit to Capital Account	155 732	164 929
USD	365 822	361 409

Affiliate Membership Programme Income and Expenses

Income	1995	1994
Contributions[21]	67 544	75 338
Royalties Blackwell	3038	2309
Ties & Scarves	580	273
Transfer from General Income & Expenses	10 800	1981
Debit to Capital Account	1539	0
USD	83 501	79 901

Expenses	1995	1994
IUPAC Secretariat (AMP)	28 877	27 360
Chem. Intl. & Leaflets	51 686	49 309
Miscellaneous Expenses	2938	3232
USD	83 501	79 901

Notes to Accounts

1. Accounting Policies

a. Basis of Preparation of Financial Statements

The financial statements are prepared under the historical cost convention.

b. Tangible Fixed Assets and Depreciation

Tangible fixed assets are stated at cost less depreciation. Depreciation is provided on all tangible fixed assets at rates calculated to write off the cost less estimated residual value of each asset on a straight-line basis over its expected useful life as follows:

Fixtures and fittings—over 5 years

Computer hardware—over 5 years

c. Leasing Commitments

Rentals paid under operating leases are charged to the Income and Expenses account on a straight line basis over the period of the lease.

d. Foreign Currencies

Transactions in foreign currencies are recorded at the rate ruling at the date of the transaction. Monetary assets and liabilities are retranslated at the rate of exchange ruling at the balance sheet date. All differences are taken to the income and expenses account, except those incurred in investment transactions, which are taken direct to the balance sheet.

e. Investments

Interest on investment bonds is recognized on a receipts and not an accruals basis.

f. Committed Expenses

The IUPAC Council meets once every two years at the General Assembly to agree budgets for committee operations for the following two years. Starting in 1994, seventy per cent of the budgeted expenses is charged to the income and expenditure account in the first year following the General Assembly and thirty per cent in the General Assembly year.

g. Royalty Income

Royalty income is recognized in the income and expenditure account on a cash received basis.

h. Legal Status

The official headquarters of IUPAC are in Zürich, and the legal domicile of the Union is accepted by the Canton of Zürich as an association under Swiss Law. As such the Union is exempt from any taxation on any net income arising from its activities.

2. Accounts Payable	1995	1994
List Oxford	27 462	23 654
List New York	7170	–
	34 632	23 654

3. Provisions and Subaccounts	1995	1994
Committed Expenses	0	76 072
Bad Debts	9062	19 950
CHEMRAWN Conference Loan Fund	7654	15 839
Neutra/Audit	9000	8000
Purchases from Blackwells	500	564
Royal Society Contbn. to Dev. Activs.	11 145	19 922
Kratos Grant	136	136
ICSU Grants	32 408	35 184
Lewis Publishers	5004	5004
UNESCO grants	130	0
Organic Synthesis	1523	1523
Destruction of Chemical Weapons	4621	6434
Oxford University Press —Solubility Data Series	6193	2286
	87 376	190 914

4. Prepaid Subscriptions	1995	1994
Croatia NAO 1996	1000	–
Czech Republic NAO 1996	1300	–
Eurachem AO 1996	50	–
ICCC AO 1996	50	–
IZA AO 1996	100	–
Egypt CA 1996	450	–
Hungary CA 1996	450	–
Hungary CA 1997	450	–
Hong Kong OC 1996	50	–
Netherlands NAO 1995	–	18 100
ICC AO 1995	–	50
IOCG AO 1995	–	50
Netherlands CAs 1995	–	450
Egypt CA 1995	–	450
Poland CA 1995	–	450
Russia CA 1995	–	450
Thailand CA 1995	–	450
Bulgaria OC	–	200
	3900	20 650

5. Capital Gains Realized	1995	1994
Capital Gains Realized	–32 137	–25 493
Gain on Building Fund	7993	0
Exchange Differences on Building Fund	6225	0
	–17 919	–25 493

6. Fixed Assets	1995	1994
Fixed Assets	95 529	91 586
Depreciation of Assets over 5 Years	–73 027	–54 241
	22 502	37 345

7. Cash in Banks

	1995	1994
USD	4190	28 291
GBP	15 999	13 949
CHF	0	65
East European Banks (arrangements are in hand to close the Czechoslovakia bank account)	17	517
Money Market Investments	387 022	822 465
	407 228	865 287

8. Marketable Securities

The Marketable Securities are stated at book value in 1994 and at market value in 1995, following a decision by the IUPAC Finance Committee (Minute 4.1(ii)/96, Zürich).

	1995	1994
Book Value	1954 365	1500 642
Unrealized Profit	89 381	–71 169
Market Value	2043 746	1429 473

9. Building Fund

On the recommendation of the IUPAC Council (Minute 7/91, 36th Meeting—Hamburg), part of the Union's assets have been moved into a building fund, to provide for the eventuality that the need for a permanent Secretariat building becomes pressing.

10. Accounts Receivable

	1995	1994
List Oxford	13 485	10 029
List New York	9883	–
	23 368	10 029

11. Subscriptions, etc., Outstanding

	1995	1994
National Organizations	36 250	62 637
Observer Country Service Charges	0	0
Company Associates Service Charges	0	100
Associated Organization Service Charges	0	100
	36 250	62 837
National Organizations (1993)		
Chile	0	1800
Egypt	0	3800
		5600
National Organizations (1994)		
Argentina	0	1100
Belgium	0	18 200
Chile	0	2600
Egypt	0	5500
Greece	0	3300
Israel (CA)	0	400
Japan	0	23 187
Turkey	0	2750
		57 037
National Organizations (1995)		
Argentina	1100	–
Chile	2800	–
Egypt	5800	–
Greece	3500	–
Kuwait	700	–
Turkey	5650	–
USA	16 700	–
	36 250	
Service Charges Company Associates (1994)		
Israel	0	50
USA	0	50
Service Charges Associated Organizations (1994)		
FECS	0	50
IFCC	0	50

12. National Subscriptions

	1995	1994
Received	594 462	542 725
Outstanding	36 250	57 037
	630 712	599 762

13. Company Associate Service Charges

	1995	1994
Received	9000	9250
Outstanding	0	100
	9000	9350

14. Observer Country Service Charges

	1995	1994
Received	1100	650
Outstanding	0	0
	1100	650

15. Associated Organization Service Charges

	1995	1994
Received	1550	1550
Outstanding	0	100
	1550	1650

16. Office Expenses

	1995	1994
IUPAC Officers	9734	4326
IUPAC Secretariat (Non-pubns.)	269 114	272 462
Audit, Bank Fees, Other Charges	12 059	35 517
	290 907	312 305

17. Expenses IUPAC Bodies

	1995	1994
Administration Expenses	39 642	14 306
Meetings other than General Assembly	104 698	203 022
Transfer to CHEMRAWN Account	0	11 100
General Assembly	329 411	7901
	473 751	236 329

18. Bad Debts Write Off

	1995	1994
Bulgaria (AMP)	–44	44

19. Other Expenses

	1995	1994
Contributions to ICSU	19 785	18 857
Representatives Other Organizations	6560	8007
IUPAC Handbook 1994–1995	15 654	0
Chem. Intl. for Members	21 481	21 195
Publicity Brochures	0	12 233
Appointment of Information Officer	3180	8297
Miscellanous Expenses	11 439	3713
Transfer to Affiliates in Developing Countries	10 800	1981
	88 899	74 283

20. Miscellaneous Expenses	1995	1994
BS Travel Grant	20 000	20 000
Other	9774	5535
	29 774	25 535

21. AMP Contributions	1995	1994
In USD	66 990	75 338
From East Europe	554	0
	67 544	75 338

Securities Account as at 31 December 1995

	Currency	Amount	Approx. price %	Market value (USD)	Book value at cost	Profit/(loss) since purchase (potential)
Bonds						
6.5% Toyota	USD	100 000	101.13	101 125.00	97 009.72	4115.28
6 3/8% ABB Internat Finance	USD	100 000	100.06	100 062.00	97 634.38	2427.62
7% Chubu Electric Power Co. Inc	USD	100 000	100.31	100 312.00	99 019.44	1292.56
5 7/8% Euro Ciba-Geigy 1993—23.3.2000	USD	100 000	100.81	100 812.00	100 260.00	552.00
5.5% General Electric 1993—8.4.1998	USD	150 000	100.31	150 468.00	152 280.56	–1812.56
5.75% Osaka Gas 1993—26.5.1998	USD	100 000	100.50	100 500.00	104 428.40	–3928.40
Certificates of Deposit						
CD Republic NB New York	USD	50 000	100.03	50 015.00	50 051.78	–36.78
Mutual Funds						
Haussmann Holdings	USD	370	775.45	286 916.50	239 356.70	47 559.80
ML Basic Value	USD	14 780	19.51	288 357.80	236 723.87	51 633.93
ML Euro Equity	USD	12 842	15.86	203 688.11	200 792.32	2895.79
ML Pacific Equity	USD	13 000	9.73	126 490.00	126 475.70	14.30
Aetna European Equity	USD	11 700	11.64	136 188.00	143 012.61	–6824.61
Meridian Global Government Fund	USD	4500	10.85	48 825.00	50 490.00	–1665.00
Meridian US Emerging	USD	9067	21.38	193 859.72	197 813.00	–3953.28
Permal Asian Holdings	USD	55	1073.02	56 126.95	59 016.64	–2889.69
Grand Total Securities				2043 746.08	1954 365.12	89 380.96

Recent Reports

In this section we publish summaries of the most recent IUPAC recommendations on nomenclature and symbols and technical reports. The full texts of these recommendations and reports are published in *Pure & Appl. Chem.*

Pesticides report 34. Pesticide runoff: Methods and interpretation of field studies (Technical Report)

Synopsis: The objectives, design and interpretation of experimental measurements of pesticide losses in rainfall-induced runoff from the surfaces of agricultural fields are reviewed. Microplot- and Mesoplot-scale experiments (which use artificial rainfall), and field- and watershed-scale experiments (which use natural rainfall), provide different but complementary information. The smaller-scale experiments are more controlled, replicable and easier to undertake but cannot represent those processes which vary over larger scales; thus they may not be representative of many real situations. Larger-scale field and watershed monitoring experiments provide realistic runoff concentrations, but they are more difficult and expensive. Because rainfall is uncontrolled, they are likely to provide unrepresentative data which are difficult to interpret and to extrapolate to other field and weather scenarios. A risk-of-runoff assessment of a pesticide may require information from a combination of these tests, together with the use of computer simulations to integrate the results.

This report has been prepared for publication by R.D. Wauchope[1], R.L. Graney[2], S. Cryer[3], C. Eadsforth[4], A.W. Klein[5] and K.D. Racke[3] ([1]US Department of Agriculture, Agricultural Research Service, Tifton, GA, USA; [2]Bayer Agricultural Division, Stillwell, KS, USA; [3]DowElanco Corp., Indianapolis, IN, USA; [4]Shell Research Ltd, Sittingbourne, Kent, UK; [5]Umweltbundesamt, Berlin, Germany) of the Commission on Agrochemicals of the Applied Chemistry Division.
The full details are to be found in Pure Appl. Chem. *1995, **67**, 2089–2108.*

Pesticides report 35. Offsite transport of pesticides in the aqueous phase: Mathematical models of pesticide leaching and runoff (Technical Report)

Synopsis: The process of modelling the leaching and runoff of pesticides is simple in concept but complex in execution. Models are physical, conceptual, or mathematical representations of reality. Screening-level models are an appropriate first step for examining pesticide leachate and runoff potential, as long as conservative input assumptions are used. They may consist of comparisons of certain mobility and persistence properties with numerical criteria, or they may require pencil, paper, and a hand calculator. At a higher level of sophistication, a wide variety of computer models are available that can quantitatively simulate pesticide leaching and runoff in the aqueous phase. It is important to pick a model that has been validated in more than one study, has good user support, requires a quantity of data input appropriate for the application, and has a history of producing results acceptable to scientists and regulatory authorities. Considering these various criteria for acceptability, EPA's PRZM2 model and the German modification, PELMO, would be appropriate for evaluating leaching potential. The GLEAMS, LEACEIM, and CALF models are also scientifically acceptable, but have not been as widely used. The GLEAMS model is appropriate for quantifying runoff potential in simple, field-scale drainage patterns. The more complex SWRRBWQ model is more appropriate for watershed-scale assessments. The most appropriate use of these computer simulations is to rank the contamination potential of a particular pesticide at several sites, or to rank several pesticides at one site. Another excellent application of these models is to calibrate them to fit the results of an intensive field study at one site, and extrapolate to other points in time and space for the same pesticide. One should always recognize the variability of natural processes and field conditions, and use probabilistic (stochastic) analysis whenever possible. More model validation and calibration is needed in tropical climates and in special situations such as turf, forests and orchards.

This report has been prepared for publication by S.Z. Cohen[1], R.D. Wauchope[2], A.W. Klein[3], C.V. Eadsforth[4] and R. Graney[5] [with acknowledgements to J. Lin (Bayer-USA), T. Durborow (E&TS-USA) and R.D. Jones (EPA-USA)] (Environmental & Turf Services, Inc. Wheaton, Maryland, USA; [2]Agricultural Research Service, USDA, Tifton, Georgia, USA; [3]Umweltbundesamt, Berlin, Germany; [4]Shell Research Ltd, Sittingbourne, Kent, UK; [5]Miles/ Bayer, Inc., Stilwell, Kansas, USA) of the Commission on Agrochemicals of the Applied Chemistry Division. Full details are to be found in Pure Appl. Chem. *1995, **67**, 2109–2148.*

A glossary of terms used in chemical kinetics, including reaction dynamics (IUPAC Recommendations 1996)

Synopsis

This Glossary is a compilation of terminology recommendations in the field of chemical kinetics. Every effort has been made to include what appear to be the most commonly accepted definitions. It is hoped that the Glossary will be a helpful guide to those who are writing books and articles in the field. The reader is warned, however, that alternative definitions of some of the terms, such as Adiabatic and Rate-Controlling Step, are frequently to be found in the scientific literature.

This Report was prepared for publication by Keith J. Laidler (Department of Chemistry, University of Ottawa, Ottawa, Ontario KIN 6N5, Canada) for the Subcommittee on Symbolism and Terminology in Chemical Kinetics of the Physical Chemistry Division. The full details are to be found in Pure Appl. Chem. *1996, **68**, 149–192.*

High resolution wavenumber standards for the infrared (Technical Report)

Synopsis

The calibration of high resolution infrared spectra is generally more precise than accurate. This is the case even when they are recorded with Fourier transform interferometers. The present document aims at improving the accuracy of wavenumber measurements in the infrared by recommending a selection of spectral lines as wavenumber standards for absolute calibration in the range from about 4 to about 7000 cm^{-1} The uncertainties of these wavenumber standards range from $\pm 1 \times 10^{-3}$ to $\pm 1 \times 10^{-6}$ cm^{-1}. Sources of frequency standards, on which the wavenumber determinations are based, are also given

This Report was prepared for publication by G. Guelachvili[1], M. Birk[2], Ch.J. Bordé[3], J. W. Brault[4], L. R. Brown[5], B. Carli[6], A. R. H. Cole[7], K. M. Evenson[8], A. Fayt[9], D. Hausamann[2], J. W. C. Johns[10], J. Kauppinen[11], Q. Kou[1], A. G. Maki[12], K. Narahari Rao[13], R. A. Toth[5], W. Urban[14], A. Valentin[15], J. Vergès[16], G. Wagner[2], M. H. Wappelhorst[14], J. S. Wells[8], B. P. Winnerwisser[17], M. Winnerwisser[17] ([1]Laboratoire de Physique Moléculaire, CNRS UPR-136, Université Paris-Sud, Bâtiment 350, 91405 Orsay-Cedex, France. [2]1nstitute for Optoelectronic, DLR, D-82234, Wessling, Germany. [3]Laboratoire de Physique des Lasers,

Université Paris-Nord, Avenue Jean Baptiste Clément, 93430 Villetaneuse, France. [4]NoAA Aeronomy Lab. R/E/AL5, 325 Broadway, Boulder, Co, 80303, USA. [5]Jet Propulsion Laboratory, California Institute of Technology, Pasadena, 91109, USA. [6]Istituto de Ricerca sulle Onde Elettromagnetiche del CNR, Via Panciatichi 64, 50127 Firenze, Italy. [7]School of Chemistry, The University of Western Australia, Nedlands, W. A. 6009, Australia. [8]NIST, Time and Frequency Division, 325 Broadway, Boulder, Colorado 80303, USA. [9]Molecular Spectroscopy Laboratory, Catholic University of Louvain, B 1348 Louvain-la-Neuve, Belgium. [10]Steacie Institute for Molecular Sciences, National Research Council, 100 Sussex Drive, Ottawa, KIA OR6, Canada. [11]University of Turku, Department of Applied Physics, FIN-20500 Turku, Finland. [12]Department of Chemistry, University of Washington, Seattle, Washington 98195, USA. [13]The Ohio State University, Department of Physics, 174 West 18th. Avenue, Columbus, Ohio 43210-1106, USA. [14]1nstitut für Angewandte Physik der Universität Bonn, Wegelerstrasse 8, 53115 Bonn, Germany. [15]Lab. de Physique Moléculaire, CNRS UPR-136, Université P. et M. Cune, 4 Piace Jussieu, 75252 Paris-Cedex 05, France. [16]Laboratoire Aimé Cotton, Bâtiment 505, 91405 Orsay-Cedex, France. [17]Physikalisch-Chemisches Institut, Justus-Liebig-Universität Giessen, Heinnch-Buff-Ring 58, 35392 Giessen, Gerrnany) for the Commission on Molecular Structure and Spectroscopy of the Physical Chemistry Division. The full details are to be found in Pure Appl. Chem. *1996, **68**, 193–208.*

The advent of high resolution Fourier transform interferometers has considerably improved the quality of the measurement of line profiles, and in particular the determination of their spectral positions. The wavenumbers of the rovibrational lines of the 2–0 band of CO were proposed as standards in 73Gue with a derived value of the velocity of light, considered as a good check of the accuracy of these data. Additional checks, bringing additional confidence, were performed by comparing the positions of the lines of the 10 mm band 00^01–$[10^00,02^00]$ Π of CO_2 measured by heterodyne techniques (74Pet) and by the same Fourier transform interferometer (82Gue). One year later heterodyne measurements were made on the 2–0 band of CO (83Pol), and Fourier spectra of the 10 mm band of CO_2 and of the 1–0 band of CO (83Jen) were recorded. These two independent experiments revealed that the claimed accuracy of the previously given Fourier wavenumber standards was overestimated, and that they had to be slightly lowered by about 0.5×10^{-3} cm^{-1}. This was confirmed in 1985 by an extensive Fourier transform experiment (85Bro) where more details about these developments can be found.

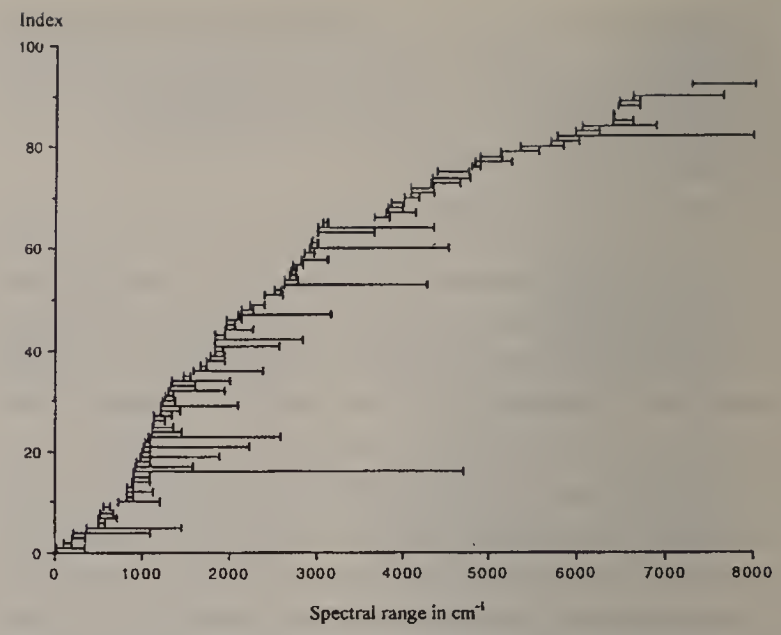


Fig. 1 Spectral range and coverage over the infrared and far infrared for the different frequency standards discussed in the Report of Guelachvili *et al*.

These discrepancies between measurements from several sources have long been unexplained. This is one of the essential reasons why the present IUPAC working group 'Unified Wavenumber Standards' was constituted in order to provide accurate wavenumber standards by combining complementary talents and tools to track the systematic errors. Extensive heterodyne frequency and Fourier wavenumber measurements have been performed. Independent measurements of the same spectral features and critical comparisons of the various softwares used for their data processing have been realised. Also, the instrumental origins of the initial discrepancies are now better understood (90Kou). The result of this work is that the wavenumber standards presented in this document are given with uncertainties ranging from $\pm 1 \times 10^{-3}$ to $\pm 1 \times 10^{-6}$ cm^{-1}.

News

Groundwater contamination

The pollution of groundwater supplies is of importance for us all whether in developed or developing countries. IUPAC has had a long tradition of experts investigating the origin and nature of contaminants in groundwater supplies. For example, in 1987 a report from the Commission on Pesticide Chemistry detailed a number of conclusions.

Potential Contamination of Groundwater by Pesticides, IUPAC Reports on Pesticides (no. 23), Prepared for publication by N. Aharonson (Institute of Plant Protection, Agricultural Research Organization, Bet Dagan, Israel) for the Commission on Pesticide Chemistry of the Applied Chemistry Division of IUPAC.

The objectives of this review were to summarize existing information on the occurrence of pesticides in groundwater and processes resulting in their detection, to identify existing technologies, and to describe missing information needed to make assessments and predictions.

Validated data on the occurrence of pesticides in groundwater are still limited. Pesticides can reach groundwater following normal agricultural usage and improper disposal and handling. Three frequently detected pesticides—aldicarb, atrazine and DBCP—are considered in detail, while other reported occurrences are summarized. Stability and transformation processes that determine the amount of a pesticide actually reaching groundwater are described. Transformation processes include microbial metabolism and chemical reactions. While these processes are well researched for the root zone, less data are available on the subsoil and saturated zone. Other factors influencing the rate and amount of pesticide infiltration include the soil–subsoil–groundwater structure, depth of groundwater, macropore flow, and rainfall or water management practices.

An attempt is made to quantify the pesticide properties and field conditions to predict their potential for leaching. Experimental and mathematical models are described and the importance of well defined field studies is emphasized.

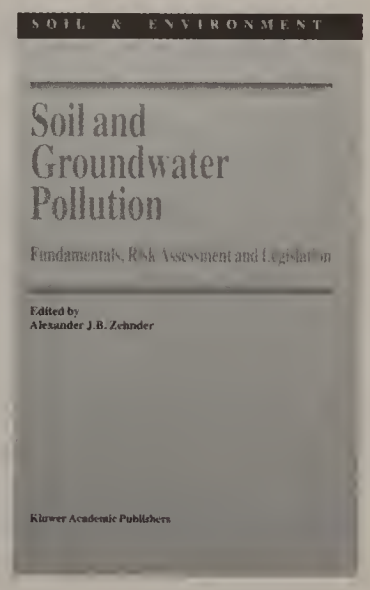
For many years the likelihood of contamination of groundwater by synthetic organic chemicals was largely ignored. The assumption that the soil profile always serves as an efficient purifying filter led to the conclusion that extensive penetration of pollutants into ground water was unlikely. Recent reports on groundwater contamination, however, aroused public and government concern about a potential threat to the quality of drinking water. Indeed, in 1981 experts speculated that in the USA almost 1% of groundwater resources contain detectable amounts of foreign organic chemicals. This figure may be misleading, however, since the contamination is usually associated with populated areas and therefore probably has a proportionally greater impact on drinking water supplies.

In contrast to previous assumptions, groundwater quality may be affected by human activities, particularly by the widespread use of organic chemicals. Under certain soil and climatic conditions, some organic compounds exhibit sufficient soil mobility and persistence to allow them to reach groundwater; the recent discovery of aldicarb and other carbamates—as well as some halogenated hydrocarbons and triazines— has been confirmed in some groundwater. The extent of occurrence of pesticides in ground water is still unknown, however, and the magnitude of the problem has to be defined. Preliminary findings indicate a need for more monitoring to determine the extent of the problem and interdisciplinary research to elucidate the processes governing the transport and fate of organic chemicals in subsoil and groundwater.

The full details of this report may be found in *Pure Appl. Chem.* 1987, **59**,1419–1446.

In a similar vein the following book has recently been published by SCOPE (Scientific Committee on Problems of the Environment, established by ICSU in 1969) working with UNEP (United Nations Environmental Programme) and the Swiss Federal Institute for Environmental Science and Technology (EAWAG).

Soil and Environment, Volume 4. Soil and Groundwater Pollution: Fundamentals, Risk Assessment and Legislation



SCOPE, the Scientific Committee on Problems of the Environment, was established by the International Council of Scientific Unions (ICSU) in 1969 as an international, nongovernmental, nonprofit organization with the mandate to:

—advance knowledge of the influence of humans on their environment, as well as the effects of these environmental changes upon people, their health and their welfare, with particular attention to those influences and effects which are either global or shared by several nations;

—to serve as a non-governmental, interdisciplinary and international council of scientists and as a source of advice for the benefit of governments and intergovernmental and nongovernmental bodies with respect to environmental problems.

SCOPE has been established because critical environmental concerns call for a thorough evaluation of the issues at stake, an assessment of their consequences at global and regional levels and the formulation of possible solutions.

Through its activities, SCOPE identifies available knowledge, then synthesizes it to point out where gaps

and uncertainties exist, and to recommend where efforts should be concentrated to develop explanations and solutions.

SCOPE aims at the dissemination of information to as wide an audience as possible and to communicate it in a readily understandable form for practitioners in the scientific community and also for policy planners and decision makers, industry managers, engineers, technicians, teachers, and the public at large. It is only through such action that sound policies can be adopted to prevent, mitigate or adapt to the effects of an existing or potential environmental problem.

Groundwater pollution as a result of soil pollution has long been treated as a minor problem, either because the necessary analytical methods were not available or because the extent of the pollution was largely underestimated. It was only after the Love Canal incident in the late 1970s in the USA, and soon afterwards at Lekkerkerk in the Netherlands, that world-wide authorities, and scientists for groundwater and soil pollution have taken interest in groundwater pollution. In 1987, SCOPE decided that an expert group should deal specifically with this problem, taking into account the special needs of the different regions of our globe.

This workshop and symposium in Cesky Krumlov, is one of a series. The first workshop took place in Stanford, California, USA, the second in Bangkok, Thailand, and the third in San José, Costa Rica. More are planned, one in Beijing, China and the other in Adelaide, Australia. This is the fourth; it specifically focused on soil and groundwater pollution in Central and Eastern Europe. It was the first workshop and symposium which took, besides scientific, legal and risk issues into account. These issues are necessary for a successful implementation of protection and remedial measures.

The aim of the workshop and symposium was to bring together scientists, engineers, lawyers, authorities and private enterprises to discuss new developments in legislation and in remediation and prevention measures against soil and groundwater pollution, and to make recommendations for future developments in technology, science and regulations.

Soil and Groundwater Pollution, edited Alexander J.B. Zehnder; Kluwer Academic Publishers, PO Box 17, 3300 AA Dordrecht, the Netherlands (1995); xi + 164 pp., ISBN 0 7923 3743 3.

Names and Addresses

Full details (names, addresses, telephone/telex/Fax numbers and E-mail) of the officers of IUPAC bodies were published in *Chemistry International* 1995, **17**(6), 215–226. The IUPAC Secretariat have been notified of the following changes:

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Dr P. Dysseler (Chairman, Commission VI.6), E-mail: dysseler@meurice.indutec.technopol.be

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Dr Barry J. Whyte (Secretary, Nomenclature Committee of IUBMB (NC-IUBMB) and IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN)) Editorial Office, European Journal of Biochemistry, Kleinstrasse 6, Postfach, CH-8032 Zürich, Switzerland; Tel.: +41 1 268 1150; Fax: +41 1 268 1151; E-mail: whyte@biocfebs.unizh.ch

Provisional Recommendations

IUPAC seeks your comments

In this section we publish synopses of IUPAC's latest provisional recommendations on nomenclature and symbols. All comments on these recommendations are welcome and will be taken into consideration. The final revised versions are published in *Pure and Applied Chemistry* and synopses of these are published in *Chemistry International* as recent reports.

If you would like to comment on the provisional recommendations please write to your nearest national/regional centre requesting a copy of the full report. Copies are not available from the IUPAC Secretariat. The most recent list of the national/regional centres appeared in *Chemistry International* 1995, **17**, 141.

Glossary of terms used in bioinorganic chemistry

The glossary contains definitions and (where needed) explanatory notes for about 400 terms used in the multidisciplinary field of bioinorganic chemistry. A need has been recognized for globally acceptable definitions of terms in this field and this glossary was compiled with the objective of fulfilling this need. It is by no means a comprehensive dictionary. The terms selected were those considered essential and/or widely used. The definitions given reflect current usage and complement IUPAC guidelines. Abbreviations and acronyms, frequently used in bioinirganic chemistry, are included.

Comments on these recommendations are welcome and should be sent by 30 November 1996 to: Dr M.W.G. de Bolster, Vakgroep Organizche en Anorganizche Chemie, Faculteit der Scheikunde, Vrije Universiteit, De Boelelaan 1083, 1081 HV Amsterdam, the Netherlands, Fax: +31 (20) 444 7488.

ISO Standards

The following are some of the new international standards announced by the International Organization for Standardization (ISO) in recent issues of *ISO Bulletin*.

New international standards published between 11 November 1995 and 13 December 1995:

TC 28	**Petroleum products and lubricants**
ISO 7536:1994**	Petroleum products—Determination of oxidation stability of gasoline—Induction period method
TC47	**Chemistry**
ISO 10143:1995	Carbonaceous materials fot he production of aluminium—Calcined coke for electrodes—Deterination of the electrical resistivity of granules
ISO 10236:1995	Carbonaceous materials fot the production of aluminium—Green coke and calcined coke foor electrodes—Determination of bulk density (tapped)
TC 156	**Corrosion of metals and alloys**
ISO 10270:1995	Corrosion of metals and alloys—Aqueaous corrosion testing of zirconium alloys for use in nuclear power reactors
TC 190	**Soil quality**
ISO 11269-2:1995	Soil quality—Determination of the effects of pollutants on soil flora—Part 2: Effects of chemicals on the emergence and growth of higher plants

New international standards published between 14 December 1995 and 11 January 1996:

TC 45	**Rubber and rubber products**
ISO 249:1995	Rubber, raw natural—Determination of dirt content
ISO 1409:1995	Plastics/rubber—Polymer dispersions and rubber latices (natural and synthetic)—Determination of surface tension by the ring method
ISO 1433:1995	Rubber, vulcanized—Preferred gradations of properties
ISO 2302:1995	Isobutene–isoprene rubber (IIR)—Evaluation procedures
ISO 2398:1995	Rubber hose, textile-reinforced, for compressed air—Specification
ISO 3900:1995	Rubber—Nitrile latex—Determination of bound acrylonitrile content
ISO 8030:1995	Rubber and plastics hoses—Method of test for flammability
ISO 11234:1995	Rubber compounding ingredients—Carbon black (pelletized)—Determination of dust content
TC 61	**Plastics**
ISO 1147:1995	Plastics/rubber—Polymer dispersions and synthetic rubber latices—Freeze-thaw cycle stability test
ISO 1163-1: 1995	Plastics—Unplasticized poly(vinyl chloride) (PVC-U) moulding and extrusion materials—Part 1: Designation system and basis for specifications

ISO 8618:1995	Plastics—Liquid phenolic resins—Conventional determination of non-volatile matter
ISO 8619:1995	Plastics—Phenolic resin powder—Determination of flow distance on a heated glass plate
ISO 8987:1995	Plastics—Phenolic resins—Determination of reactivity on a B-transformation test plate
ISO 8989:1995	Plastics—Liquid phenolic resins—Determination of water miscibility
ISO 11567:1995	Carbon fibre—Determination of filament diameter and cross-sectional area
ISO 12992:1995	Plastics—Vertical flame spread determination for film and sheet
TC 107	**Metallic and other inorganic coatings**
ISO 2723:1995	Vitreous and porcelain enamels for sheet steel—Production of specimens for testing
ISO 10308:1995	Metallic coatings—Review of porosity tests
TC 146	**Air quality**
ISO 6879:1995	Air quality—Performance characteristics and related concepts for air quality measuring methods
TC 147	**Water quality**
ISO 10712:1995	Water quality—Pseudomonas putida growth inhibition test (Pseudomonas cell multiplication inhibition test)
ISO 11734:1995	Water quality—Evaluation of the 'ultimate' anaerobic biodegradability of organic compounds in digested sludge—Method by measurement of the biogas production
TC 190	**Soil quality**
ISO 10573:1995	Soil quality—Determination of water content in the unsaturated zone—Neutron depth probe method

New International Standards published between 12 January 1996 and 10 February 1996:

TC 45	**Rubber and rubber products**
ISO 1656:1996	Rubber, raw natural, and rubber latex, natural—Determination of nitrogen content
ISO 8054:1996	Rubber, compounded or vulcanized—Determination of sulfide sulfur content—Iodometric method
TC 147	**Water quality**
ISO 5667-1:1980/ Cor 1:1996	Technical Corrigendum 1
ISO 6107-1:1996	Water quality—Vocabulary—Part 1
ISO 6107-5:1996	Water quality—Vocabulary—Part 5
ISO 6107–6:1996	Water quality—Vocabulary—Part 6

New International Standards published between 11 February 1996 and 14 March 1996:

TC 27	**Solid mineral fuels**
ISO 333:1996	Coal—Determination of nitrogen—Semi-micro Kjeldahl method
ISO 351:1996	Solid mineral fuels—Determination of total sulfur—High temperature combustion method
ISO 609:1996	Solid mineral fuels—Determination of carbon and hydrogen—High temperature combustion method
ISO 625:1996	Solid mineral fuels—Determination of carbon and hydrogen—Liebig method
TC 28	**Petroleum products and lubricants**
ISO 6614:1994**	Petroleum products—Determination of water separability of petroleum oils and synthetic fluids
TC 147	**Water quality**
ISO 6341:1996	Water quality—Determination of the inhibition of the mobility of Daphnsa magna Straus (Cladocera, Crustacea)—Acute toxicity test

** French version of standard previously published in English only

Full details of these and other ISO standards may be obtained from: ISO Central Secretariat, Case Postal 56, CH-1211 Geneva, Switzerland. Tel.: +41 22 749 01 11; Fax: +41 22 733 34 30.

Use of the World Wide Web for access to IUPAC documents

Use of the Internet, and particularly the World Wide Web, has been expanding at an enormous rate—see the report on the UNESCO/ICSU sponsored conference on electronic publishing earlier in this issue. While it is clear that IUPAC must make use of this new, and widely effective, mode of communication, it is less clear exactly how best to use it. The Committee on Printed and Electronic Publications (CPEP) was asked both to establish the Home Page and to suggest guidelines for the use of those committees and individuals in IUPAC who have information (both 'official' and unofficial) to disseminate.

In drawing up these guidelines, the CPEP has tended to stress open and free (no-cost) distribution over pay-per-view or access limited to those who have paid for the print equivalent. In so doing, the CPEP recognizes that it may, over time, be necessary to protect the revenue of IUPAC's printed publications through more restricted access to some of the Web pages. Nevertheless, at this early stage of our experience with electronic distribution, we have thought it preferable to encourage very broad usage, so that both the Union and chemists world-wide have incentive to learn how to use this exciting new medium to advantage.

1.0 Material published in *Chemistry International*

In principle, any material published or due to be published in *Chemistry International* may be displayed at the IUPAC Web site (at present maintained by the Royal Society of Chemistry at Pipex, Cambridge, UK;

URL http://chemistry.rsc.org/rsc/iupac.htm), at the discretion of the IUPAC Information Officer.

2.0 Recommendations published in *Pure & Applied Chemistry*

In principle, all recommendations and technical reports published in *Pure & Applied Chemistry* will be made freely available via the World Wide Web, by one of the following methods.

2.1 The file should preferably be mounted at the IUPAC Web site either as part of the directly available HTML-formatted Web material or in a separate directory accessible to ftp. To facilitate these arrangements, the document author should provide the computer-readable version, with a description of the file type (e.g. HTML or Microsoft Word RTF) at the same time as final camera-ready copy is submitted to *Pure & Applied Chemistry*.

2.2 Alternatively, the file can be mounted by the author or an associate at his/her local site as a fully HTML-formatted Web document.

An example is the Glossary of Class Names mounted at Queen Mary and Westfield College, London. In this case the IUPAC Web Home Page will contain a hypertext link to the appropriate URL address (e.g. http://www.qmw.ac.uk/~ugca000/iupac.html). Full reference should be made to the original publication and the IUPAC copyright statement should be included. Initially, documents made available in this way should be transferred eventually to the IUPAC Web site, in order to ensure their long-term availability.

2.3 The file can be held in native word-processor or compound document format (compressed if appropriate) at the local site, and made available for transfer by FTP. The IUPAC Web Home Page will contain a hypertext ftp link to the file.

3.0 Recommendations on nomenclature and symbolism published in compendium form (the IUPAC Colour Books)

This is material from which IUPAC expects to derive income from hard-copy sales. Recommendations not previously published in *Pure & Applied Chemistry* can be made available as outlined in sections 2.1–2.3, but not until 12 months after publication of the book.

4.0 Provisional recommendations

Past experience with IUPAC drafts has shown that provisional recommendations are often used by the community regardless of their status. The possibility of making such drafts more widely available by the use of the Internet should therefore be viewed with caution. However, the advantages of reaching a wider community for review of drafts are considerable. The following arrangements will therefore be made.

4.1 The IUPAC Web site will display titles and synopses of provisional recommendations (as published in *Chemistry International*) as HTML files. Those requiring a copy of the draft (on Paper) will be instructed to send a request to the appropriate regional document distribution centre at the address given: where possible this will be facilitated by an e-mail–hypertext link. All distribution drafts should carry the prominently displayed message: Provisional Recommendations—FOR COMMENT ONLY, NOT TO BE CITED, on each page.

4.2 In addition, at the discretion of the Chairman of the Commission concerned, the document may be mounted as a native or HTML file at the author's local site as outlined in section 2.2, with a hypertext link from the displayed title and synopsis on the IUPAC Home Page. If a document is made readily available for downloading in this way, its provisional status should be made clear by the prominently displayed message: Provisional Recommendations—FOR COMMENT ONLY, NOT TO BE CITED, on each page. This message should appear as a 'watermark' (preferred) or as text inserted at frequent intervals.

5.0 Pre-provisional draft recommendations

IUPAC will make available joint publications in the ways outlined in sections 2.0 and 3.0 provided that all the material concerned is IUPAC-approved. Hypertexted links from the IUPAC Home Page will be given for material at sites maintained by other organizations. In cases where joint publications contain material not approved by IUPAC or outside its control, this fact will be made clear in the specification of the hypertext link.

6.0 Pre-provisional draft recommendations

Some Commissions and Working Parties will wish to use the World Wide Web as a medium for the circulation of and comment on draft material at an earlier stage, before submission to IDCNS. This is potentially a valuable means of facilitating input to IUPAC proposals, and will be allowed at the discretion of the Commission Chairman. However, such an arrangement should be managed via facilities available to Commission members, without involving the IUPAC Web site. Documents mounted on the Web in this way should be clearly marked with a draft number and date, and each page should carry the prominently displayed text: DRAFT FOR COMMENT: NOT TO BE CITED.

Password-protection facilities should be used if available, to ensure that access is restricted to members of the group concerned. Text in such drafts should avoid phraseology susceptible to extraction and quotation out of context as IUPAC recommendations (e.g. IUPAC-approved values are...).

Recommendations prepared by Dr Alan McNaught, Secretary, IDCNS.

New Publications

Macromolecular Symposia

The 35th International Symposium on Macromolecules sponsored by the International Union of Pure and Applied Chemistry was held on July 11–15, 1994 at the University of Akron, in Akron, Ohio, USA

The scientific programme of this meeting was divided into 11 sections and 24 subsections:

1. Plenary Lectures

2. New Polymerization Reactions and Reaction Mechanisms
Radical Polymerization; Ionic Polymerization of Olefins and Heterocyclics; Metathesis and Coordinative Polymerizations; Metal Catalysed and Other Chain and Step Polymerizations;

3. Complex Macromolecular Architecture and Supramolecular Polymers
Liquid Crystals; Helices and Dendrimers; Macrocyclics, Rotaxanes and Molecular Recognition; Nanoarchitectures;

4. Polymers and Biology
Biocatalytic Synthesis; Biomedical Polymers;

5. Frontier Polymeric Materials
Composites and Networks; Inorganic/Organic Hybrids; Fluorinated Polymers; Degradation and Recycling;

6. Field Responsive Polymers
Conducting and Electroluminescent Polymers; Nonlinear optical Polymers; Ferroelectric/Piezoelectric Polymers;

7. Structure and Morphology
New Imaging and Other Techniques; Scattering Techniques in Amorphous and Ordered Polymers;

8. Thermodynamic and Dynamic Properties in Solution and Bulk
Spectroscopic Probes and Molecular Modelling; Rheological and Rheooptical Behaviour; Phase Transitions;

9. Polymers at Interfaces
Configuration, Morphology and Modelling at Interfaces; Microrheology at Interfaces;

10. History of Polymers

11. Industrial Views on Polymers in the 21st century
This Symposium was attended by 1700 participants from 47 countries. Five Plenary and 131 Invited Lectures were presented during this meeting. The lectures have been printed as an especially large volume of the series: *Macromolecular Symposia*, Vol. 98.

One particularly thought provoking paper presented at this meeting is entitled:

In Search of the Plastic Enzyme, by J.E. Guillet, N.A. D. Burke, Maria Nowakowska*, Howard Reese and D.M. Gravett (Department of Chemistry, University of Toronto, Toronto, Canada M5S IA1)

**Permanent address: Faculty of Chemistry, Jagellonian University, Krakow, Poland.*
Enzymes, which have remarkable catalytic properties, are unique macromolecular species synthesized by living organisms. Typically they are assembled from a variety of amino acid residues into polymers with molecular weights ranging from about 2 to 100 kilodaltons and with a very well defined geometry, particularly in the region of the active site, where chemical reaction occurs. Unlike most active catalysts used in conventional synthetic organic chemistry, they perform their catalytic functions in aqueous solutions or gels, frequently in the presence of oxygen and a variety of other reactive species of natural or biological origin.

Furthermore, it is a requirement for the chemistry of living systems that they react with a limited set of substrates with great selectivity to produce a well defined product with close to zero by-products.

The difficulty of meeting this formidable set of requirements in a single macromolecule has been a major deterrent to the initiation of research programmes to produce a truly synthetic enzyme, which uses the same chemical principles but nonbiological intermediates in its construction.

Over the past decade, the above research group has been studying the catalytic properties of some unusual macromolecules which mimic some of the properties of natural enzymes. These water soluble molecules, which are composed primarily of copolymers of hydrophobic and hydrophilic monomers are powerful catalysts which sensitize a wide range of photochemical reactions in water with considerable selectivity and

specificity. The authors term them 'photozymes' (photochemical enzymes).

Although most natural enzymes do not sensitize photochemical processes, the use of light permits a sophisticated probe of the kinetics and mechanism of chemical reactions in enzyme models which, hopefully, can provide information useful in designing more advanced polymeric catalysts for thermal reactions as well.

Photozymes

Photozymes possess several interesting properties: (1) water solubility, (2) solubilizing ability, (3) absorbance of the ultraviolet portion of the sunlight spectrum, and (4) efficient transfer of photochemical energy collected over a large volume of the polymer to a dissolved molecule. Thus aqueous solutions of photozymes will dissolve more of a sparingly water-soluble compound than would dissolve in water alone and the compound is located preferentially within the polymer coils. Upon irradiation, dissolved molecules undergo efficient photoreactions.

Recent studies carried out by the above authors have focused on the preparation, characterization and photocatalytic properties of water-soluble copolymers with covalently attached aromatic chromophores. Hydrophobic interactions between the aromatic chromophores and water result in the formation of hydrophobic microdomains. Sparingly water-soluble organic compounds are readily solubilized within these microdomains. The high local concentration of aromatic chromophore found along the polymer backbone results in efficient light-harvesting systems in which the energy of photons absorbed at sites remote from a solubilized molecule may migrate through the polymer and be transferred to the solubilized molecule. The polymers have been shown to act as sensitizers for a number of different photochemical reactions in aqueous solution: photooxidation of polycyclic aromatic hydrocarbons, photodechlorination of polychlorinated biphenyls, photohydroxylation of styrene, photolysis of undecanone, and photoisomerization of 7-dehydrocholesterol to previtamin D_3.

Synthesis

Photozymes can be prepared by radical copolymerization of two (or more) vinyl monomers. The final polymer must have enough hydrophobic nature that it will have solubilizing ability, but not so much that it is insoluble in water. Typically, several mixtures of monomers are polymerized and the polymer with the best properties is selected for further study.

In most of this work, photozymes were synthesized by radical copolymerization of a hydrophobic and a hydrophilic monomer. One of the monomers, usually the hydrophobic one, bears a chromophore with appropriate photophysical and photochemical characteristics. The bulk of the polymers used in this work were prepared using sodium styrenesulphonate, although many other hydrophilic monomers could be employed (i.e. acrylic acid or vinylbenzoic add).

The principal means of varying the properties of the photozymes is by changing the nature of the chromophore on the hydrophobic monomer. By changing the chromophore, it is possible to have photozymes which absorb visible or deep UV light, sensitize singlet or triplet reactions, and act as electron donors or acceptors.

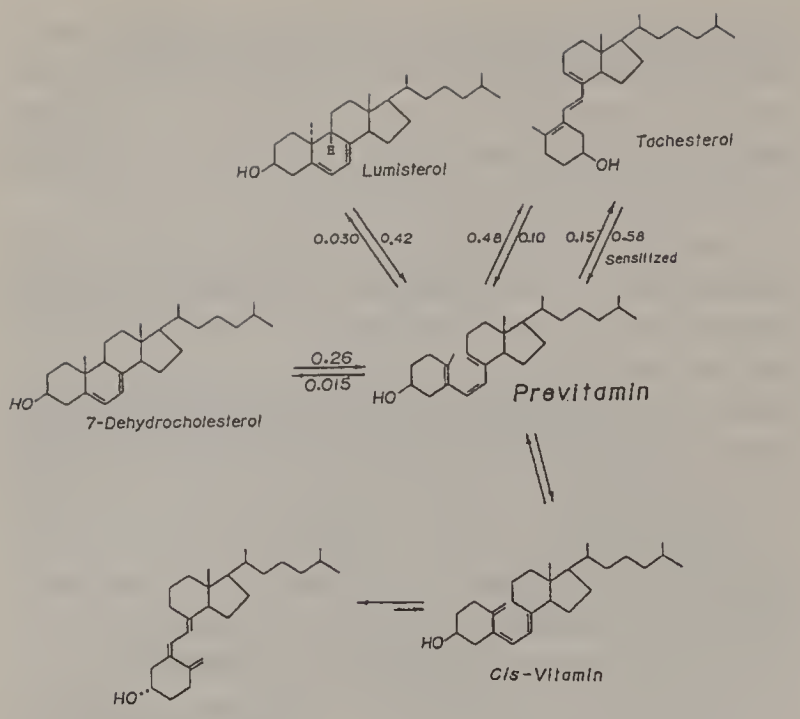
As examples of the potential use of these photozymes consider the following two examples. Firstly the photodechlorination of chlorinated aromatics and secondly the solar synthesis of previtamin D_3.

Previously these authors have reported that certain photozymes are effective catalysts for the photodechlorination and thus detoxification of polychlroinated benzenes in natural sunlight. This work has now been extended to heaxchloro- and pentachlorobenzenes (HCB and PeCB, respectively). The distribution of HCB between water and the polymer phase in aqueous photozyme solution was estimated by using a solid-phase extraction technique that has been used previously to determine the binding (solubilization) of hydrophobic molecules by humic materials. The partition coefficient for HCB and PeCB were shown to be of the order of 10^5–10^6, similar to those for PCBs and polycyclic aromatic hydrocarbons.

The rates of dechlorination in aqueous solutions of both PSSS-VN and poly[(sodium *p*-styrenesulphonate)-co-(acenaphthylene)](PSSS-AcN) in simulated sunlight were at least a thousand times greater than in organic solvents. Photodechlorination was slower in organic solvents, even when 2-methylnaphthalene was present at the same concentration as the naphthyl chromophores in PSSS-VN solution.

These results confirm the potential for the elimination of chlorinated organics in water by treatment with catalytic photozymes in solar ponds or by high-intensity UV lamps. Photodechlorination of PeCB in photozyme solutions leads to the preferential formation of 1,2,4,5-tetrachlorobenzene.

By analogy with the perylene photooxidation the authors suggest that this very rapid dechlorination occurs, possibly through an exciplex intermediate, via electron transfer from naphthalene (or acenaphthene) to HCB or PeCB. The resulting radical anion of the chlorinated organic splits out a chloride ion into water, and the resulting radical fragment removes a hydrogen atom from a hydrogen-donating substance. The process is sequential as the chlorine atoms are removed from the aromatic rings one at a time, and continue until virtually no chlorine is left.



Scheme 1.

As with perylene photooxidation, the polymer can play an additional role in the reaction. The photozymes have a powerful means of separating the ion pair. The photozyme bears many negatively charged groups (sulphonate anions) so there will be a considerable repulsive force between the photozyme and the radical anion. If the ion pair is forced apart by the electrostatic forces within the photozyne then it is much more likely that dechlorination will be observed at the expense of back electron transfer.

The photochemistry of the isomers belonging to the Vitamin D family has been the subject of extensive studies for many years. This attention reflects the important biological and medical roles these compounds play. The synthesis of Vitamin D is one of the few examples of photochemical reactions of commercial importance. However, until recently, the yields of photochemical conversion were restricted to about 30% because the products of the irradiation of 7-dehydrocholesterol (DHC) absorbed light more strongly than DHC itself, and continued reaction formed various byproducts which were not biologically active.

The most important reactions, based on studies reported by Jacobs and Uavinga, are illustrated in Scheme I. The numbers associated with the arrows represent the relevant quantum yields. The overall process involves two steps: the first photochemical, the second thermal. In the first step the starting material, DHC, undergoes photochemical conrotatory ring opening of the cyclohexadiene system to form the Z-hexatriene derivative, previtamin D, which can then be thermally converted to *cis*-Vitamin D by a reversible 1.7 H-shift. Unfortunately, the previtamin also undergoes a photochemically induced back ring closure, which both regenerates DHC and creates the 9,10 anti-isomer side product, lumisterol. It also displays $Z \rightarrow E$ photoisomerization to the 6–7 isomer, tachysterol. All these photochemical reactions are reversible and all, except $Z \rightarrow E$ isomerization, can occur in the corresponding molecule only through the first excited singlet state. The $Z \leftrightarrow E$ photoisomerization which interconverts previtamin and tachysterol can occur both in the singlet and in the triplet states of these molecules. Because intersystem crossing in alkenes is very inefficient, the triplet state can only be significantly populated by energy transfer from a properly chosen donor.

Another article which appeared in this current volume which has an appropriately thought-provoking title was *Molecular architecture for the Twenty First Century—New products from old monomers*, by O. W. Webster (Du Pont Central Research and Development, Experimental Station, PO Box 80328, Wilmington, DE 19880-0328, USA)

Twentieth century polymers have been used primarily to fill space, i.e. they are valued for their physical properties. Twenty-first century polymers will be valued for their chemical properties as well. For clues as to what these chemical properties will be, we can look to nature. In the 20th century we have copied and sometimes bettered nature's ability to fill space with polymers (silk, cotton, wool, sea shells, wood, hair, and bone) but we have only begun to mimic her chemical use of polymers (enzymes, hormones, and DNA for example).

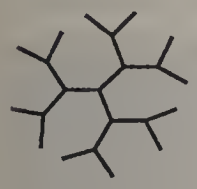
To synthesize polymers with unusual properties from the existing basic monomers (a necessity for commercial success) one needs to place the monomer units in ordered arrays rather than at random as in the old methods of synthesis. Thus polymer architecture control is a rapidly expanding area for research.

Homopolymers

The synthesis of linear homopolymers has progressed from random coil architectures to helices to bundles of rigid rods and on to narrow molecular weight dispersity polymers by living polymerizations. In the next century, exact molecular weight polymers patterned after nature's synthesis of proteins will most likely abound. With respect to synthetic linear exact molecular weight polymers, Rothe has made a polyproline 40mer, and polyethylene of up to 195 units has been prepared. Seebach is presently synthesizing pure poly(3-hydroxybutyrate) of 64 and 96 units to study its bioactivity—apparently in most living cells there are traces of this polymer–ion channels in the cell walls. What is badly needed for exact molecular weight polymer synthesis is a switching mechanism (thermo for example) so that one could rapidly add monomer units one at a time to growing polymer chain ends.

In the rapidly expanding area of dendritic polymers pioneered by Tomalia, all of the diverse polymers reported have been designed to have exact molecular

weights. Dendritic polymer, **4**, based on ethylenediamine and methylacrylate, has been made shell-wise up to molecular weights in the 100 000s. During synthesis the molecular weight, which is more or less exact, doubles with the formation of each shell. DSM sells a dendritic amine based on step-wise cyanoethylation with acrylonitrile and hydrogenation. Similar hyperbranched polymer can be made by polym-



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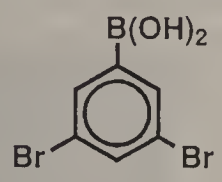

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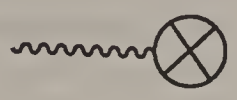

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erization of A_2B type monomers such as **5** but the branching and molecular weights are not exact.

Combination of dendritic and other globular polymers with linear polymer chains has given polymer architec-

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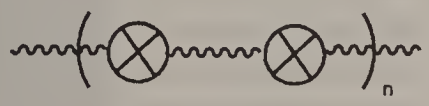

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ture a new dimension. Tadpole-shaped polymer, **6**, has been reported, bolo polymer, **7**, and bead polymer, **8**. Cyclic polymers, **9**, made by coupling reactive double-ended living polymers have been known for some time now. Cyclic oligomers have been used as monomers for synthesis of the corresponding linear polymers by ring opening polymerization. Since the bonds in the cyclic oligomer are the same as those in the linear polymer there is little density change on polymerization—a useful property. Several unusual cyclic ribbon macro-

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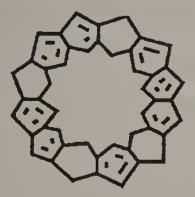

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molecules, **10**, have been synthesized by cycloaddition reactions. In other work, involving large rings, chain structures, **11**, and rings threaded on a polymer chain, **12**, have been made.

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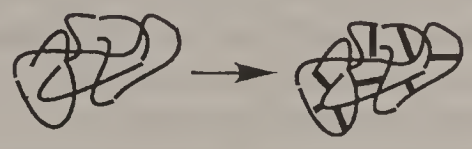
Polymerization of bisvinyl monomers usually results in a crosslinked gel. If the spacing between the vinyl units is 2 or 3 atoms, cyclic polymerization gives a loop polymer, **13**. Larger loops can be formed if dilute conditions are employed. Indeed when linear polystyrene of molecular weight 300 000 was cross-linked by alkylation at 0.5% concentration (w/w), all of the crosslinks formed intramolecularly to make a modified loop polymer, **14**, with no change in molecular weight.



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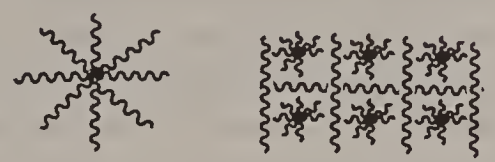
Addition of divinyl monomer to active-ended polymer generated by living polymerization produces a soluble star polymer, **17**, that has as many as 200 arms radiating from a crosslinked core. Simms finds that crosslinking hard star polymer into a regular acrylic coating gives a bead polymer network, **18**, that is both hard and flexible, properties that are difficult to obtain in the same film.



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Block polymers

Soon after linear synthetic polymers were discovered it was noted that very few pairs formed uniform mixtures. Due to their high molecular weights the entropy of mixing is low. Thus polymers do not dissolve in each other unless functional group interactions are high. To get around this disturbing feature one can hook the two polymer chains together to form a block copolymer. The polymers will still phase-separate but only into microdomains of spheres, cylinders, or lamellae. Depending on the molecular weight of the copolymer and relative block sizes either block can be the continuous phase.

Block polymers are synthesized by addition of a second monomer to reactive polymer formed by a living polymerization or by connecting reactive ended segments through a condensation reaction. In this manner AB, ABA (AB)X, ABC, and in at least one case, ABCD block polymers have been made. In the next century the different architectural forms of block polymers will continue to expand as researchers combine the block polymer concept to the known architectural forms of homopolymers: stars, dendritic, hyperbranched, cyclic,and networks. The number of different monomers that can be included in block polymers will continue to expand. The change in properties related to sequence order will be interesting. How will the properties of ABCD polymer differ from those of ADCB, etc.?

The junction between the blocks can be sharp or tapered, i.e. contain both monomers. An interesting case of a tapered block polymer is one in which each chain starts out with monomer A and gradually increases the

amount of B until it ends with pure B. The most interesting block polymers have blocks with greatly different block properties, for example, hydrophobic/hydrophilic, fluorocarbon/hydrocarbon, ionic/nonionic, and crystalline/amorphous blocks. The use of blocks made up of random copolymers greatly increases the property variations available from block polymers.

Some notable uses for block polymers are dispersing agents, non-ionic detergents, and thermoplastic elastomers. Kraton®, themoplastic rubber, and Lycra® spandex fibre, are two well known commercial block polymers.

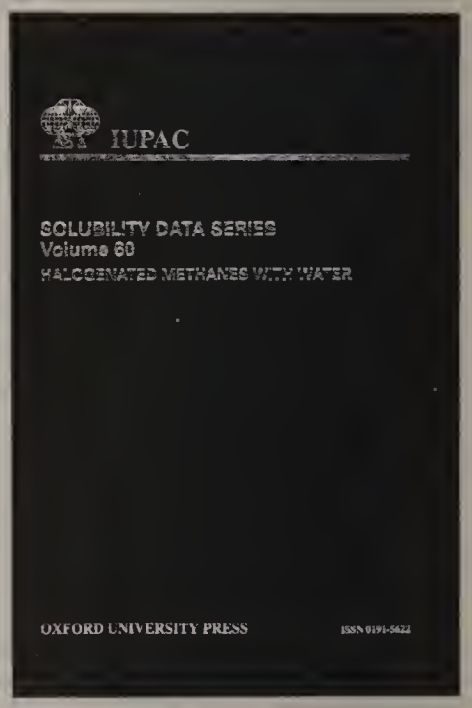
Supramolecular assemblies

An area of intense interest lately is supramolecular assemblies, wherein a number of molecules combine through hydrogen bonding, electrostatic attraction or hydrophobic interaction to form large arrays. Some examples are: liquid crystalline polymers, spherical micelles (from single-chain lipids with large ionic head groups), cylindrical micelles (from single-chain lipids with small ionic head groups) and vesicles (hollow bilayer systems from double-chain lipids with large ionic head groups). Hydrogen bonding between carboxylic groups or isocyanurates and melamine are ideal ways to assemble supramolecules.

Solubility Data Series, Volume 60. Halogenated Methanes with Water

This volume and the forthcoming supplements, *Halogenated Ethanes and Ethylenes with Water* and *Halogenated Aliphatic Compounds C3–C14 with Water*, contain compiled solubility data from the published literature through to the end of 1992. All the collected data were critically examined for their reliability and best value estimates were selected on the basis of such evaluations. Reported and best value data are given in tabular form, and, where justified, data correlation equations and graphical illustrations are provided. Throughout the volume, SI conventions have been employed as the customary units.

The halogenated aliphatic compounds of this volume are of particular interest and concern for engineers, scientists, health workers and the general public because of the extensive use of such materials in industrial and agricultural applications. Currently, attention has been focused on actual and potential hazards of the halogenated hydrocarbons. The emphasis is mainly related to the destruction of ozone in the stratosphere and the carcinogenic effect of halocarbons on the human population. Information on the solubility of the halogenated aliphatic hydrocarbons is needed so that their expected concentrations in the stratosphere, drinking water, foodstuffs, human tissue, marine organisms, and the like can be determined with reasonable certainty.



Halogenated Methanes with Water (Volume 60 of the Solubility Data Series) was edited by Ari L. Horváth and Forrest W. Getzen and published by Oxford University Press, Walton Street, Oxford OX2 6DP, UK (Tel.: +44 (0)1865 267907), 1996: xix + 197 pp. ISSN 0191 5622.

Solubility Data Series, Volume 61. Alkali Metal and Ammonium Perchlorates: Part I. Lithium and Sodium Perchlorates.

The alkali metal and ammonium perchlorates form an interesting group in that the lithium and sodium salts

IUPACSEARCH Version 4.1

Free computer disks containing all IUPAC recommended nomenclature and symbols and technical reports published in *Pure and Applied Chemistry* from 1960 through the end of 1994 are now obtainable from the IUPAC Secretariat. The disks are 3½ in., high-density, IBM-PC compatible format and will run under DOS (version 3.3 or later), a Windows version is in preparation. A hard disk with 5 Mb of free space and 640 kb or greater of RAM are required. The software is easy to use and allows for Boolean searches; it is menu-driven and easy to use. Both colour and mono monitors are supported. Sorry, a Macintosh version is not available.

Please E-mail or Fax your request to: Mrs Gwyneth Pettit, Fax: +44 (0)1943 880310; E-mail: acadsoft@bcs.org.uk

are very soluble in water and are hydrated, while the ammonium, potassium, rubidium and caesium salts have low solubilities and are unhydrated. Lithium and sodium perchlorates are also much more soluble in nonaqueous solvents than the other perchlorates.

Volume 61: Part I contains critical evaluations and solubility data for lithium and sodium perchlorates in all solvents and in all systems at different temperatures, compiled from recognized publications, many of which are of Russian origin and often not readily accessible. This volume will be followed by Part II which will contain data on potassium, rubidium, caesium and ammonium perchlorates.

Literature coverage is complete up to the end of 1991. The original data have been recalculated to conform to IUPAC-recommended units, but both original and recalculated data are presented. Data for solubilities in many solvents other than water have been compiled, e.g. lithium perchlorate in 61 other solvents, sodium perchlorate in 17 and potassium perchlorate in 32 other solvents. The alkali metal perchlorates have wide applications, ranging from the widespread use of the more soluble perchlorates as supporting electrolytes, to the use of the potassium and ammonium salts in the manufacture of explosives and solid rocket propellants and the lithium salt as a battery electrolyte. These volumes are of use to physical scientists and engineers in many different fields, both in industry and in academic and research institutions.

Alkali Metal and Ammonium Perchlorates: Part I. Lithium and Sodium Perchlorates (Volume 61 of the Solubility Data Series) was edited by C.Y. Chan, K.H. Khoo, E.S. Gryzlova and M.-T. Saugier-Cohen Adad and published by Oxford University Press, Walton Street, Oxford OX2 6DP, UK (Tel.: +44 (0)1865 267907). 1996; xviii + 268 pp. ISSN 0191 5622.

Solubility Data Series, Volume 62. Carbon Dioxide in Water and Aqueous Electrolyte Solutions.

Four volumes of the Solubility Data Series on the solubility of carbon dioxide have been either published or planned. The first was published four years ago (Vol. 50, *Carbon Dioxide in Non-aqueous Solvents at Pressures under 200 kPa*, edited by Peter G.T. Fogg).

The present volume will be followed by two volumes, one on the solubility of carbon dioxide in aqueous organic solvents at all temperatures and pressures and another on solubility of carbon dioxide in nonaqueous solvents at partial gas pressures greater than 200 kPa.

The systems carbon dioxide + water and carbon dioxide + aqueous electrolytes are of great importance in the environment, as well as in physiology, biology, geology and industrial applications, not least because the solubility of carbon dioxide in water is an order of magnitude larger than that of many simple gases.

For this volume, the scientific literature has been searched systematically, starting historically with the work of Bunsen (1855) and including most articles published up to the end of 1994. The volume contains compilations of solubility data for carbon dioxide in water, water-D_2O (heavy water), sea water, and aqueous electrolyte solutions at temperatures between 268 and 773 °K and pressures up to 3 kbar. About 85% of the data sets presented are for pressures less than 2 bar. The electrolytes comprise approximately 70 different salts and their mixtures. Data for 125 systems and 260 data sets have been evaluated critically on the basis of the total carbon dioxide dissolved, regardless of the species present in solution. Because of the large amount of data, certain systems have been excluded from the volume, for example, carbon dioxide in biological fluids such as blood, and in beer, wine and soft drinks. Alkaline systems have also been excluded.

Carbon Dioxide in Water and Aqueous Electrolyte Solutions (Volume 62 of the Solubility Data Series) was edited by P. Scharlin and published by Oxford University Press, Walton Street, Oxford OX2 6DP, UK (Tel.: +44 (0)1865 267907). 1996; xvii + 383 pp. ISSN 0191 5622.

The Solubility Data Series has been published as a journal by Oxford University Press since 1994, and a discount of 25% for both a subscription (four issues) and individual volumes applies to all IUPAC members,including members of IUPAC Commissions and Committees, and Affiliates. The price to IUPAC members for a subscription is GBP 199/USD 296 (compared to the full price of GBP 265/USD 395). For individual volumes, IUPAC members may purchase these for GBP 60/USD 90 each (compared to the full price of GBP 80/USD 120). Please note that Sterling rates apply in UK and Europe; United States dollar rates apply elsewhere.

Molten Salts Bulletin *'Sels Fondus'*

The latest bulletin in this series, 1996 No.59, has just been published and contains a recent bibliography and details of recent conferences and publications devoted to the study of molten salts. To continue this series of publications, interested readers are requested to send information and reprints concerning their work in this field to:

Molten Salts Bulletin Sels Fondus, M. Gaune-Escard, Institut Universitaire des Systèmes Thermiques Industriels, UA 1168, Université de Provence, Centre St. Jérôme, 13397 Marseille Cedex 20. France.

Conferences

International Conference on Chemical and Biological Thermodynamics, Amritsar, India, 5–8 January 1997

IUPAC SPONSORED

This conference is intended to review advances in basic and applied thermodynamics in the following areas:

- Non-reactive systems
- Critical fluids
- Phase transitions
- Interfacial phenomena
- Ligand binding processes
- Energetics of biological systems
- New techniques

Golden Temple (Amritsar)

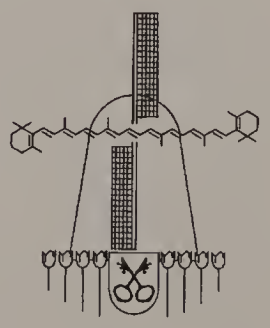
The registration fee is USD 300 before 30 September 1996, USD 350 after 30 September 1996, for active participants, and USD 120 before 30 September 1996, USD 150 after 30 September 1996, for students. This registration fee will include a registration package, morning tea/coffee, working lunch and afternoon tea for the duration of the conference.

For further information, please contact: Prof. Bhajan Singh, Department of Chemistry, Guru Nanak Dev University, Amritsar-143005, India. Fax: +91 183 258 820; E-mail: bhajan@gndu.ernet.in

11th International Symposium on Carotenoids, Leiden, the Netherlands, 18–23 August 1996

IUPAC SPONSORED

In 1966, an International Symposium on Carotenoids was held in Trondheim, Norway. This proved to be the first in a series of successful meetings, held every three years under the auspices of IUPAC. The 11th meeting in this series is to be held at Leiden, the Netherlands, those interested in any area of carotenoid science, academic or commercial, are cordially invited to participate and to present a paper.



The registration fee is NLG 500 for active participants, and NLG 150 for nonscientific participants.

For further information, please contact: Secretariat of the 11th International Symposium on Carotenoids, Prof. Dr J. Lugtenburg, Chairman, PO Box 9502, 2300 RA Leiden, Netherlands. Tel.: +31 71 527 4405; Fax: +31 71 527 4537; E-mail: lugtenbu@chem.leidenUniversity.nl

8th International Conference on Bioinorganic Chemistry (ICBIC8), Yokohama, Japan, 27 July–1 August 1996

IUPAC SPONSORED

The scientific programme will been organized around five daily plenary lectures. These plenary lectures will introduce topics which will be expanded upon by the invited speakers in subsequent sessions, and in poster presentations. It is hoped that there will be ample opportunity for informal exchange of ideas.

Topics to be discussed include:

- Metal recognition, storage and transport
- Structure and function of the active sites of metalloenzymes
- Industrial applications of bioinorganic chemistry
- Electron transfer
- Nitrogen and nitric oxide biochemistry
- Metals in medicine
- Metals and nucleic acids
- Environmental bioinorganic chemistry

The registration fee is JP¥ 60 000 for active participants, JP¥ 40 000 for students and JP¥ 20 000 for nonscientific participants. This registration fee includes a copy of the Abstracts, refreshments, a get-together party and banquet.

For further information, please contact: Prof. Masanobu Hidai, Chairman, ICBIC 8, Department of Chemistry and Biotechnology, Graduate School of Engineering, University of Tokyo, Hongo, Bunkyo-ku, Tokyo 113, Japan. Tel.: +81 3 3812 2111 ext 7261; Fax: +81 3 5800 6945

Discovery of the Elements, Leuven, Belgium, 17–20 September 1996

The initiative for this symposium was taken by the Katholieke Universiteit Leuven to celebrate the scien-

tific heritage of Walter and Ida Noddack. The programme of this meeting will cover both the science involved in the discovery of the elements and the history of this science. In details, the meeting will address:

- Survey of ancient discoveries
- 19th century discoveries
- Recent discoveries
- Elements in stars
- Artificial elements (fission-related and others)
- Noddack-devoted session (rhenium, masurium/technetium and fission)
- General, for example, criteria for identifying and naming elements

These topics cover a large number of scientific disciplines, mostly at the limits of contemporary technology. The organizers hope that the meeting will focus on demonstrating how the discoveries of new elements pushed the developing technology.

The registration fee is BEF 10 000, this includes symposium services, Proceedings and social programme.

Details about this meeting may be found on the Internet at: http://www.fys.kuleuven.ac.be/iks/elem.html, and from: Dr Pieter Van Assche, Westerlosesteenweg 3, B-2230 Herselt, Belgium, Tel.: +32 14 54 02 64; Fax: +32 14 54 16 88; E-mail: pva@innet.be

9th IUPAC International Congress on Pesticide Chemistry, London, UK, 2–7 August 1998

IUPAC SPONSORED

Two keynote lectures will be given by Sir Colin Berry and Prof. Hubert Markl at the formal opening session. The Congress will cover the following topics:

- Environmental fate
- Synthesis and SAR
- Metabolism
- Regulation and risk assessment
- Delivery
- Resistance and mode of action
- Residues in food and environment
- Natural products

The meeting will be a mixture of plenary lectures and parallel sessions, with invited oral contributions and posters. The fees for attendance have not, as yet, been finalized, but it is likely that the conference fee will be in the range GBP 250–350 for participants and GBP 100–150 for students.

For further information, please contact: Dr John F. Gibson, 9th IUPAC International Congress—Pesticide Chemistry, The Royal Society of Chemistry, Burlington House, London W1V 0BN. Tel.: +44 171 437 8656; Fax: +44 171 734 1227

36th IUPAC Congress, Geneva, Switzerland, 17–22 August 1997

IUPAC SPONSORED

The New Swiss Chemical Society and the Organizing Committee hereby send a cordial invitation for the 36th IUPAC Congress, Geneva, 17–22 August 1997. This Congress will provide an ideal opportunity for academic and industrial chemists, from around the world, to exchange ideas and experience on topics related to the general theme *Frontiers in Chemistry: New Perspectives for the 2000s*. The aim of the organizers is to bring together distinguished experts not only to present their own work, but to discuss the major scientific and technological challenges facing chemistry in the next millenium.

The conference programme will include Plenary Lectures, Section Keynote Lectures, Invited and Contributed Oral Papers and Poster Presentations. The Scientific Committee has selected the following interdisciplinary themes that will provide a framework for lectures and discussions:

- Advanced materials
- Catalysis and synthetic methods
- Molecular properties and reaction pathways
- Medicinal chemistry and combinatorial chemistry
- Supramolecular chemistry and biomolecular recognition
- Advances in computational chemistry
- Chemistry and society

These themes will be presented concurrently in five parallel sessions in the traditional fields of: Organic Chemistry, Inorganic Chemistry, Physical and Technical Chemistry, Analytical chemistry and Nanosciences, and Chemistry and Biology.

IUPAC NSCS

The following scientists have agreed to give plenary lectures:

G. Balavoine (France)
P. J. Crutzen (Germany)
G. Ertl (Germany)
O. Kahn (France)
J. Nüesch (Switzerland)
D. Seebach (Switzerland)
P.G. Schultz (USA)
C. Weissmann (Switzerland)
R. N. Zare (USA)

The second circular will be available in September, 1996, and will contain the full programme, together with

registration forms and details of costs. This second circular may be obtained by contacting:

36th IUPAC Congress, c/o AKM Congress Service, PO Box 37, CH-1218 Le Grand Saconnex, Switzerland. Tel.: +41 22 761 1661; Fax: +41 22 761 1662

2nd International Conference on Excitonic Processes in Condensed Matter (EXCON'96), Kurort Gohrisch near Bad Schandau, Germany, 14–17 August 1996

IUPAC SPONSORED

Sixty years after the first papers on excitons by Frankel, excitonic physics has now developed into a truly interdisciplinary field. Excitons plays a key role in excitation and energy tranfer processes in many molecules, molecular aggregates and crystals, as well as in macromolecular and biological systems. Topical examples are low-dimensional, and confined systems such as conjugated polymers and quantum wells. The applications range from, for example, determining the properties of materials to investigations of the motion of DNA strands in gels. Such investigations cover enormous ranges of chemistry and physics, together with materials science, biophysics and biochemistry.

In the spirit of the first International Conference on Excitonic Processes in Condensed Matter (EXCON'94) in Darwin, this meeting intends to cover all aspects of excitonic processes occurring in:

- clusters
- molecular aggregates
- bulk semiconductors
- quantum wells and dots
- micro and nanostructures
- surfaces
- inorganic materials
- organic materials
- biological systems
- photosynthesis

The invited speakers include: V. M. Agranovich, M. Aihara, C. von Borczyskowski, D. Fröhlich, I. Ya. Fugol, R. van Grondelle, V. Hizhnyakov, K. Kan'no, J. Knoester, R. S. Knox, E. Kotomin, G. La Rocca, H. Port, J. Shah, R. Silbey, Y. Toyozawa and R. Zimmermann.

The conference will be held at the Parkhotel Gohrischer Hof in the Kurort (Spa) Gohrisch about 2 km from Bad Schandau near the river Elbe close to the boarder with the Czech Republic.

The registration fee is DEM 380 for scientific participants and DEM 200 for students. Further information about the conference may be found on the Internet at:

http://www.tu-chemnitz.de/home/schreiber/excon/excon96.html,

and from:

EXCON'96, c/o Monika Fleischer, Institut für Physik, TU Chemnitz-Zwickau, D-09107 Chemnitz, Germany. Fax: +49 371 531 3143, E-mail: excon@physik.tu-chemnitz.de

XVIth IUPAC Symposium on Photochemistry, Helsinki, Finland, 21–26 July 1996

IUPAC SPONSORED

Photochemists meet in Helsinki this Summer!

The XVIth IUPAC Symposium on Photochemistry will be held at the University of Helsinki from Sunday 21 July to Friday 26 July 1996. The capital of Finland, with its beautiful surroundings, provides ample places to visit. Adventurous participants, who would like to experience the never-setting midnight sun, should not miss the arctic safari to Lapland. Opera fans will be sure to visit the famous Savonlinna Opera Festival following the conference. You will find, perhaps to your surprise, that prices for food and accommodation are reasonable. The reduced hotel prices charged to conference participants range from about USD 40 to 100 for single rooms. The banquet, to be held at a spectacular site on the seaside, should not be missed by anyone.

The information given in the 2nd circular and news updates about the conference are available on the internet: http://www.chemres.hu/EPA/ or http://cric.chemres.hu/EPA/.

Scientific programme

The organizers highly appreciate the positive response of all the international experts which were invited to present lectures at the Symposium. Eight Plenary and fifteen Invited Lectures commence the morning and afternoon sessions. Some 25 Short Contributions will be selected for oral presentation and will be delivered in three parallel sessions in the morning sessions from Tuesday to Thursday. Two longer and two shorter poster sessions, to be held in the halls of the main building, give an excellent opportunity for presenting scientific contributions. All posters will be on exhibition during the whole conference. Three workshops will be held to invite lively discussions on applied topics of current interest.

Thanks to the success of the previous Symposia on Photochemistry this conference requires no special recommendation. The following major themes will be covered: 1. Applied photochemistry 2. Inorganic and organometallic photochemistry 3. Organic photochemistry 4. Primary photochemical processes 5. Atmospheric photochemistry 6. Photobiology and photosynthesis 7. Molecular assemblies and supramolecular photochemistry 8. Mechanistic photochemistry 9. Photoinduced electron transfer 10.

The scientific sessions of the IUPAC Symposium on Photochemistry will take place will take place in the Porthania building and in the Great Hall of the main building of the University situated at the Senate Square in the heart of Helsinki. The University's neoclassical main building was inaugurated in 1832.

Spectroscopy 11. Theoretical photochemistry.

Plenary Lectures (60 min) will be held by the following speakers:

W. Adam: About Monoradicals, Triplet Diradicals and Higher Spin States: Understanding Electronic Substituent Effects through EPR and Time-Resolved UV Spectroscopy

M. A. El Sayed: Molecular Mechanisms of the Solar-to-Electric Energy Conversion by the Other Natural Photosynthetic System

J. Michl: Spin–Orbit Coupling in Biradicals

A. Osuka: Photoinduced Electron Transfer in Synthetic Porphyrin Arrays

J.-P. Sauvage: Rotaxanes and Other Multi-Porphyrin-Arrays as Models of the Photosynthetic Reaction Centre

J. Troe: Towards a Quantitative Characterization of Photoisomerization Rates

F. Wilkinson: Quenching of Electronically Excited States by Molecular Oxygen in Fluid Solution

Porter Award Lecture

Invited Lectures (30 min) to the plenary audience will be held by:

M. Goeldner: Photoregulation of Cholinesterase Activity Using Photolabile Probes

E. Hilinski: Heavy-Atom Effects on Photochemistry in the Picosecond Time Regime

L. B.-A. Johansson: Electronic Energy Migration and Rotational Motion within Bichromophoric Molecules

J. Kelly: Photo-Induced Electron Transfer Between Metal Complexes or Dyes and DNA

M. Klessinger: Reactive Conformations in Singlet and Triplet Photoreactions

G. Lodder: Recent Developments in Vinyl Halide Photochemistry

G. Marconi: Conformational and Circular Dichroism Studies on Cyclodextrin Inclusion Complexes

M. G. Neumann: Photochemical Study of the Interactions of Surfactants with Polyelectrolytes

M. Platz: The Photochemistry of Diazirines and the Chemistry of Carbenes

G. Rist: Photo-CIDNP as a Tool to Investigate Additives

H. Roth: Photo-Induced Electron Transfer Reactions of Strained Unsaturated and Ring Systems

J. R. Scheffer: Crystal Structure-Reactivity Relationships in Solid State Organic Photochemistry

H. Shizuka: Photophysics and Photochemistry of Triplet Exciplexes

D. Stufkens: A New Series of Re- and Ru-Complexes Having a Lowest σ, π^* Excited State That Varies From Very Reactive to Very Long-Lived

H. Tomioka: Matrix Isolation Study of Reactive *o*-Quinoid Compounds; Generation, Detection and Reactions

Three Workshops will be held in parallel dealing with the topics

J.R. Bolton/A.M. Braun: Photochemical Methods for the Oxidative Degradation of Organic Pollutants

K. Dietliker/D.C. Neckers: Photopolymerization

S. Braslavsky: Time-resolved structural changes obtained from photothermal studies in solution

An evening discussion chaired by Ed Chandross will be devoted to 'The future of photochemistry'. Well over 100 abstracts have been submitted for consideration as short oral contributions. Of these, 25 will be selected for presentation and their authors will be informed in advance. Abstracts (for format specifications see 2nd circular) received by 31 May 1996 will be included in the book of abstracts. A small prize will be awarded to the best poster presentations defended by young researchers.

Registration

Registration forms have been mailed with the second circular. The registration fees for participants are: FIM 1800, for students: FIM 100, and for accompanying persons: FIM 500. Currency exchange rate: USD 0.22/ 1.00 FIM (14 March).

The Local Organizing Committee has reduced the registration fee for participants from Central European Countries (CEC) and the New Independent States (NIS) to FIM 500 with full participation rights. In order to use this possibility you should contact directly the Chairman of the Local Organization Committee.

The reception desk will be open on Sunday 21 July, at 2 p.m. and the reception party will start at 7 p.m. Further details about the arrival in Helsinki and the Conference site will be given in the third circular that will be mailed to registered participants in June. We are looking forward to welcome you in Helsinki for an exciting and stimulating conference!

Jakob Wirz

Chairman, International Organizing Committee, Institut fur Physikalische Chemie, Klingelbergstrasse 80, CH-4056 Basel, Switzerland. Tel.: +41 61 267 38 42/ Sekr: 38 00/Fax: 38 55; E-mail: wirz2@ubaclu.unibas.ch

Helge Lemmetyinen
Chairman, Local Organizing Committee, Tampere University of Technology, PO Box 541, FIN-33101 Tampere, Finland. Tel.: +358 31 316 25 65 /Fax: 21 08; E-mail: lemme@cc.tut.fi

36th IUPAC International Symposium on Macromolecules (IUPACMACRO Seoul '96), Seoul, Korea, 4–9 August 1996

IUPAC
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The 36th IUPAC International Symposium on Macromolecules will be held at Hotel InterContinental Seoul and the Korea Exhibition Center on 4–9 August 1996. This will be the second time that IUPAC sponsored meeting will be held in Seoul. The main purpose of the Symposium is to bring together the world renowned scientists and experts to share their ideas and latest information on macromolecular science and technology.

The Symposium is also a timely event to commemorate the 20th anniversary of the Polymer Society of Korea. Dr Un Young Kim, who is the chairman of the organizing committee, Prof. Jung-Il Jin, who is the programme committee chairman, and Dr Kwang Ung Kim, who is the secretary general of the Symposium, are at present working closely together with the Polymer Society of Korea (President: Dr. Suh Bong Rhee) to make the Symposium successful.

The IUPAC MACRO SEOUL '96 will have eleven different sessions in which plenary lectures, invited lectures, contributed paper presentations either in oral or in poster will cover:

1. Polymer Synthesis and Reaction
2. Polymer Structure and Properties
3. Thermodynamics and Molecular Dynamics
4. Polymer Processing
5. Polymer Blends and Composites
6. Polymer Membranes
7. Field Responsive Polymers
8. Bio-Related Polymers
9. Supramolecular Assembly and Polymer Thin Films
10. Polymers and Environment
11. Polymer Education

Six world-renowned speakers, including Nobel laureate P. G. de Gennes of France, A. Abe of Japan, J. Economy and H. Yu of the USA, G. Wegner of Germany and Jae-Kap Sung (President of LG Chemical Ltd) of Korea have been appointed to give plenary lectures to discuss and contemplate recent trends in macromolecular science and technology, as well as the paradigm for research in the area of macromolecules in the 21st century. In addition, 136 invited lectures will be presented by experts in specific areas. Over one thousand contributed papers are expected to provide recent progress on macromolecular science and technology world-wide.

In addition to the plenary, invited lectures and oral presentations, the Symposium will also feature poster sessions and technical exhibitions.

All participants will have a chance to enjoy well organized social programmes, various programmes for accompanying persons and for post-symposium tours, through which you will find the exotic oriental culture of Korea that has spanned for almost five millenniums.

The official language of the Symposium will be English. It is estimated that 1500 participants from over 70 countries will join the IUPAC MACRO SEOUL '96.

The registration fees are USD 550 for active participants and USD 100 for accompanying persons as well as students. The IUPAC *bona fide* affiliate members are entitled to 10% reduction off the regular fee. There will be a special registration fee of USD 125 applied to participants from China, former USSR and Eastern European countries.

The Organizing Committee of the IUPAC MACRO SEOUL '96 has already arranged a sufficient number of rooms at 20–40% discounted special rates in and around the symposium venue.

Korea lies in temperate climate zone and has four distinct seasons: spring, summer, fall and winter. Summer begins from June and lasts until August. The weather is expected to be sunny and humid, and temperatures will be in the range of 25–30 °C (77–86 °F) during August. It is recommended that you bring a raincoat or an umbrella in case of occasional rain.

Seoul, the capital of the Republic of Korea, with 10 million of the nation's 45 million people, is set amid mountains, with the Han River crossing the city from east to west. There are many parks, palaces, museums and temples in or near Seoul. Visitors cannot pass up the opportunity to go shopping, souvenir collecting and sight-seeing. Itaewon, Namdaemun and Tongdaemun outdoor markets are the most popular with tourists. Major tourist attractions include the Kyoungbok Palace, Seoul Tower, Secret Garden, Chongmyo Royal Ancestral Shrine, Olympic Park and a pleasure cruise on the Han River.

Seoul

Those from abroad who are interested in participating in the Symposium should have a valid passport. Delegates from some countries may not require a visa. Please consult your local Korean Embassy or Consulate Office.

For more information please contact: Dr Kwang Ung Kim, Secretariat IUPAC MACRO SEOUL '96, Division of Polymers, Korea Institute of Science and Technology, PO Box 131, Cheongryang, Seoul 130-650, Korea. Tel.: +82 2 957 6104; Fax: +82 2 957 6105; E-mail: iupacgkistmail.kist.re.kr

Conference Calendar

1996

Organic synthesis

30 June–4 July
11th International Conference on Organic Synthesis. Amsterdam, Netherlands.
Conference Secretariat ICOS–11, PO Box 1558, 6501 BN Nijmegen, Netherlands. Tel.: +31 (80) 234471. Fax: +31 (80) 601159.

Catalysis

30 June–5 July
11th International Congress on Catalysis. Baltimore, USA.
Prof. Gary L. Haller, Department of Chemical Engineering, Yale University, PO Box 208286, New Haven, CT 06520–8286, USA. Tel.: +1 (203) 432 4378. Fax: +1 (203) 432 4387

Organometallic chemistry

7–12 July
17th International Conference on Organometallic Chemistry. Brisbane, Australia.
Prof. C. Raston, Department of Chemistry, Monash University, Clayton, VIC 3168, Australia

Chemical education

14–19 July
14th International Conference on Chemical Education—Chemistry: Expanding The Boundaries. Brisbane, Australia.
Dr W. Beasley, Graduate School of Education, The University of Queensland, Brisbane, Queensland 4072, Australia

Sweeteners

14–20 July
International Symposium on Sweeteners. Jerusalem, Israel.
International Symposium on Sweeteners, PO Box 50006, Tel-Aviv 61500, Israel. Tel.: +972 (3) 5140014. Fax: +972 (3) 5175674 or 5140077. E-mail: 100274.2665@compuserve.com

(Bio)degradable polymers

15–18 July
37th Microsymposium on Macromolecules (Bio)degradable Polymers: Chemical, Biological and Environmental Aspects. Prague, Czech Republic.
Dr B. Valter, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám 2, 162 06 Prague c-Petriny, Czech Republic

Carbohydrates

21–26 July
18th International Carbohydrate Symposium. Milan, Italy.
Prof. B. Casu, Istituto di Chimica é Biochimica 'G Ronzoni', via G. Colombo 81, 20133 Milan, Italy.

Photochemistry

21–26 July
16th Symposium on Photochemistry. Helsinki, Finland.
Prof. J. Wirz, Institut für Physikalische Chemie, Universität Basel, Klingelbergstr. 80, CH-4056 Basel, Switzerland.

Solubility phenomena

22–25 July
7th International Symposium on Solubility Phenomena. Leoben, Austria.
Prof. H. Gamsjäger, Chairman 7th ISSP, Institut für Physikalische Chemie, Montanuniversität Leoben, Franz-Josef-Strasse 18, A-8700 Leoben, Austria.

Macromolecules

4–9 August
36th International Symposium on Macromolecules. Seoul, Republic of Korea.
Dr Kwang Ung Kim, Secretariat of IUPACMACRO SEOUL'96, Division of Polymers, Korea Institute of Science & Technology, PO Box 131 Cheongryang, Seoul 130-650, Korea. Tel.: +82 (2) 957 6104. Fax: +82 (2) 957 6105. E-mail: iupac@kistmail.kist.re.kr

Excitonic processes

14–17 August
2nd International Conference on Excitonic Processes in Condensed Matter (EXCON '96). Bad Schandau, Saxonia, Germany.
Prof. M. Schreiber, Faculty of Natural Sciences, Technische Universität Chemnitz-Zwickau, D-09107 Chemnitz, Germany.

Coordination chemistry

18–23 August
31st International Conference on Coordination Chemistry. Vancouver, Canada.
31st ICCC Secretariat, UBC Conference Centre, 5961 Student Union Boulevard, Vancouver, BC, Canada V6T 2C9. Tel.: +1 (604) 822 1050. Fax: +1 (604) 822 1069.

Carotenoids

18–23 August
11th International Conference on Carotenoids. Leiden, Netherlands.
Prof. J. Lugtenburg, Gorlaeus Laboratories, Faculty of Mathematics & Natural Sciences, POB 9502, 2300 RA Leiden, Netherlands. Tel.: +31 (71) 5274405. Fax: +31 (71) 5274537. E-mail: lugtenbu@chem.leidenUniversity.nl

Macromolecular condensed state

20–25 August
International Symposium on Macromolecular Condensed State. Beijing, China.
Prof. Xibai Qiu, Secretariat, ISMCS '96, Chinese Chemical Society, PO Box 2709, Beijing 100080, China. Tel.: +86 (1) 02568157/02564020. Fax: +86 (1) 02568157. E-mail: qiuxb@infoc3.icas.ac.cn

Physical organic chemistry

25–29 August
13th International Conference on Physical Organic Chemistry. Seoul, Republic of Korea.
Prof. J. Suh, Department of Chemistry, Seoul National University, Seoul 151-742, Republic of Korea. Tel.: +82 (2) 8862184. Fax: +82 (2) 8743704. E-mail: jhsuh@plaza.snu.ac.kr

Biotechnology

25–30 August
10th International Biotechnology Symposium. Sydney, Australia.
10th IBS '96 Symposium Secretariat, GPO Box 128, Sydney, NSW 2001, Australia. Tel.: +61 (2) 2622277. Fax: +61 (2) 2622323. E-mail: veckels@tourhosts.com.au

Chemical thermodynamics

25–30 August
14th IUPAC Conference on Chemical Thermodynamics. Osaka, Japan.
Prof. M. Sorai, Executive Secretary of ICCT-96, Microcalorimetry Research Centre, Faculty of Science, Osaka University, Toyonaka, Osaka 560, Japan. Tel.: +81 (6) 8505523. Fax: +81 (6) 8505526 (or 5288).
E-mail: icct96@chem.sci.osaka-u.ac.jp

Environmental biotechnology

1–4 September
International Conference on Environmental Biotechnology. Palmerston North, New Zealand.
Conference Secretary, Environmental Biotechnology Conference, Process & Environmental Technology Department, Massey University, Palmerston North, New Zealand. Tel.: +64 (6) 3505351. Fax: +64 (6) 3505654.
E-mail: g.f.withers@massey.ac.nz

CHEMRAWN IX

1–6 September
Sustainable Production, Use, Disposal and Recycling of Materials. Seoul, Korea.
Organizing Committee & Secretariat, IUPAC CHEMRAWN IX, Tongwon B/D 6th Floor, 128-27 Tangju-dong, Chongno-ku, Seoul 110-071, Korea.

Euroanalysis IX

1–7 September
Euroanaysis IX. Bologna, Italy.
Prof. L. Sabbatini, Dipartimento di Chimica, Università di Bari, Via Orabona 4, 70126 Bari, Italy. Tel.: +39 (80) 5442020/16/14. Fax: +39 (80) 5442026.

Medicinal chemistry

8–12 September
14th International Symposium on Medicinal Chemistry. Maastricht, Netherlands
Van Namen & Westerlaken Congress Organization Services, PO Box 1558, 6501 BN Nijmegen, The Netherlands. Tel.: +31 (24) 3234471. Fax +31 (24) 3601159

Food packaging

11–13 September
International symposium on Food Packaging: Ensuring Safety and Quality of Foods. Budapest, Hungary
Dr Laura Contor—ILSI Europe, Avenue E. Mounier, 83- Box 6, B-1200 Brussels, Belgium. Tel.: +32 (2) 7710014. Fax: +32 (2) 7620014.

Characterization of porous solids

15–18 September
4th International Symposium on Characterization of Porous Solids (COPS-IV). Bath, UK.
Elaine Wellingham, Conference Secretariat, Field End House, Bude Close, Nailsea, Bristol, BS19 2FQ, UK. Tel.: and Fax: +44 (1275) 853311.

Chemistry of natural products

15–20 September
20th IUPAC Symposium on the Chemistry of Natural Products. Chicago, USA.
IUPAC Symposium Headquarters, 5999 Butterfield Road, Hillside, Chicago, Illinois 60161, USA. For further details, see http://www.a2z.com/iupac20/index.html

Multiphoton processes

30 September–4 October
7th International Conference on Multiphoton Processes. Garmisch Partenkirchen, Germany.
ICOMP VII Secretariat, Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, D-85748 Garching, Germany. Tel.: +49 (89) 32905736. Fax: +49 (89) 32905200. E-mail: rwm@mpq.mpg.de

Step growth polymerization

End-September
International Symposium on Step Growth Polymerization, Related Processes and Materials. Paris, France.
Dr B. Sillion, Laboratoire de Chimie Macromoléculaire, Université Pierre et Marie Curie, 4 place Jussieu, 75252 Paris Cédex 05, France. Tel.: +33 (1) 78022078. Fax: +33 (1) 78022010.

Pesticide use and environmental safety

13–16 October
International Workshop 'Pesticide Use and Environmental Safety in Latin America'. Sao Paulo, Brazil.
Cynthia Bergamin, Departamento de Eventos da Sociedade Brasileira de Química, Caixa Postal 26.037, CEP: 05599-970, Brazil. Tel.: +55 (11) 2102299. Fax: +55 (11) 8143602. E-mail: sbqsp@quim.iq.usp.br

1997

Thermodynamics

5–8 January
International Symposium on Chemical and Biological Thermodynamics. Amritsar, India.
Prof. Bhajan Singh, Department of Chemistry, Guru Nanak Dev University, Amritsar-143005, India. Tel.: +91 (183) 258845. Fax: +91 (183) 258820. E-mail: bhajan@gndu.ernet.in

Safety in chemical production

13–17 April
3rd Iupac Workshop on Safety in Chemical Production: Environmentally sustainable Manufacture of Competitive Products. San Francisco, USA.
Dr A. M. Ford, Gulf Coast Hazardous Substance Research Centre, Lamar University, PO Box 10613, Beaumont, Texas 77710-0613, USA. Tel.: +1 409 880 8768; Fax: +1 409 880 2397.

Bioorganic chemistry

1–6 June
4th International Symposium on Bioorganic Chemistry. Biarritz, France.
Prof. A. Marquet, Université Paris URA CNRS 493, Laboratoire de Chimie Organique Biologique, Tour 44/45–4 Pl. Jussieu, 75252 Paris Cedex 05, France.

Recycling of polymers

14–17 July
38th Microsymposium on Macromolecules, Recycling of Polymers. Prague, Czech Republic.
P.M.M. Secretariat, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám 2, 162 06 Prague c-Petriny, Czech Republic. Tel.: +42 (2) 360341. Fax: +42 (2) 367891. E-mail: sympo@imc.cas.cz

Interfacial phenomena

21–24 July
17th Discussion Conference on Macromolecules surface and interfacial phenomena in Macromolecular Systems. Prague, Czech Republic.
P.M.M. Secretariat, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám 2, 162 06 Prague c-Petriny, Czech Republic. Tel.: +42 (2) 360341. Fax: +42 (2) 367891. E-mail: sympo@imc.cas.cz

Bioinorganic chemistry

27 July–1 August
8th International Conference on Bioinorganic Chemistry. Yokohama, Japan.
Prof. M. Hidai, Department of Chemistry & Biotechnology, Graduate School of Engineering, The University of Tokyo, Hongo, Tokyo, Japan.

Plasma chemistry

18–22 August
13th International Symposium on Plasma Chemistry. Beijing, China.
Prof. Cheng-kang Wu, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100080, China. Tel.: +86 (1) 2559504. Fax: +86 (1) 2559588. E-mail: nancy@sun.ihep.ac.cn

IUPAC Congress

18–22 August
36th IUPAC Congress. Geneva, Switzerland.
36th IUPAC '97, c/o AKM Congress Service, PO Box 37, CH-1218 Le Grand-Saconnex/GE, Switzerland. Tel.: +41 (22) 7611661. Fax: +41 (22) 7611662.

IUPAC General Assembly

23–30 August
39th IUPAC General Assembly. Geneva, Switzerland.
The IUPAC General Assembly is not open for general participation but restricted to members of IUPAC bodies that meet on this occasion.

THE JOURNAL OF CHEMICAL THERMODYNAMICS

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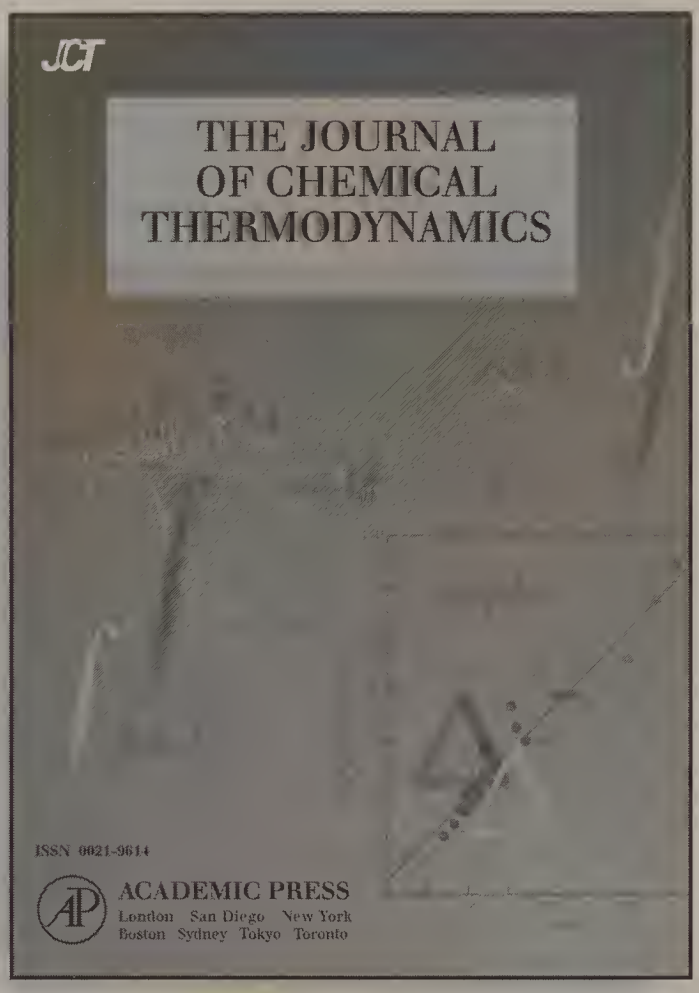

In 1996 the Journal has seen some changes: a new cover and an expansion of the scope of articles accepted for publication. The articles accepted may now encompass areas such as:

-biothermodynamics
-polymers
-phase equilibria
-interfaces
-high temperature chemistry

The Journal of Chemical Thermodynamics has established itself as the premier vehicle for the dissemination of the results of research in chemical thermodynamics. The reputation of the Journal is due in large measure to the efforts of Professor Max L. McGlashan who has served as editor for 27 years and retired from active editorial duty with the last issue of 1995.

Theoretical papers, or papers offering interpretations of experimental results previously published in the Journal, are also acceptable for submission.

While expanding the scientific base of contributions to the Journal and its readership, the Editors and Advisory Board will seek to continue the high standards and concise, elegant style upon which the reputation of the Journal has been founded.

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The International Union of Pure and Applied Chemistry (IUPAC), formed in 1919, is a voluntary non-governmental, non-profit association of organizations, each of which represents the chemists of a member country.

Its objectives are:

- to promote continuing co-operation among the chemists of the member countries;
- to study topics of international importance to pure and applied chemistry which need regulation, standardization, or codification;
- to co-operate with other international organizations which deal with topics of a chemical nature;
- to contribute to the advancement of pure and applied chemistry in all its aspects.

The membership of IUPAC presently comprises 40 countries, each represented by a national organization, such as an academy of science or research council.

National Adhering Organizations

Academy of Scientific Research and Technology **(Arab Republic of Egypt)**
Asociación Química Argentina **(Argentina)**
Australian Academy of Science **(Australia)**
Ôsterreichische Akademie der Wissenschaften **(Austria)**
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Chemistry International

IUPAC

1996, Vol. 18, No. 4 (July)

161 Changes at the IUPAC Secretariat

161 Air pollution problems in Korea
Youn Yong Lee

163 Prague Meetings on Macromolecules
Pavel Čefelín

165 Electronic publishing

169 Report of the International Union of Pure and Applied Chemistry
Mo Williams

174 IUPAC Accounts for 1995

178 Recent Reports

180 News

183 Provisional Recommendations

183 ISO Standards

184 Use of the World Wide Web for access to IUPAC documents

186 New publications

192 Conferences

197 Conference Calendar

b
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Front cover: Prof. K. I. Zamaraev, Past-President of IUPAC, who sadly died on 26 June 1996.

International Union of Pure and Applied Chemistry

Secretary General's Column

Edwin D. Becker

This is my first opportunity to communicate via this column with the hundreds of members of our Committees and Commissions, as well as the thousands of Affiliate Members. As you have doubtless read in *Chemistry International* and may have seen on the IUPAC World Wide Web Home Page, the current year has been a busy one for the IUPAC Officers and staff. The Executive Committee decided to move the Secretariat next year from Oxford to Research Triangle Park, North Carolina, USA; we are recruiting a successor to

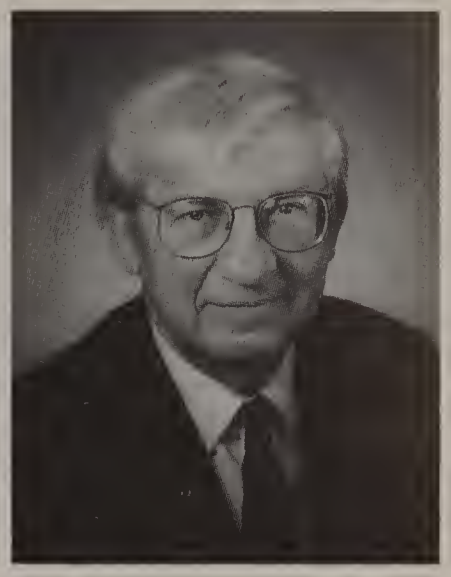
Dr Mo Williams, who will retire as Executive Secretary in April 1997; and we have been continuing to devote considerable attention to revitalizing many aspects of the Union. I will provide here some details on the rationale for recent actions and some thoughts about what we might expect to see in the near future.

Relocation of the Secretariat

The Secretariat was established in Oxford in 1968 when Mo Williams was appointed Executive Secretary. Prior to 1968 there had been no full time professional Secretariat; rather the business of the Union was conducted from the office of the Secretary General—in Paris from 1920 to 1955 under Jean Gerard and Raymond Delaby, and in Basel from 1955 to 1968 under Rudolph Morf. Initially established in Oxford as a trial locale, the Secretariat has grown and functioned well for 28 years in this location.

With the retirement last year of Miss Ann Troughton, long-time Deputy Executive Secretary, and the upcoming retirements in the next two years of Dr Mo Williams and of Mr Dass Gujral, who has been in charge of scientific publications since 1970, the Officers were led to consideration of the structure of the Secretariat and of the option to once more change location. In fact, President Fischli suggested that it might be appropriate in the present climate of rapid developments in international chemistry to review the location at regular intervals, perhaps every 10 years. Some National Adhering Organizations indicated interest in the possibility of hosting the Secretariat, and after a thorough evaluation, with much debate about the advantages and disadvantages of a move, the decision was made to accept the proposal submitted by the United States, with the location to be reassessed approximately every 10 years.

The new home of the Secretariat should be almost ideal for our needs. IUPAC will be the sole occupant of a small, one-story building in the midst of a large, heavily wooded Research Park, which accommodates research laboratories and light manufacturing for a number of international chemical, pharmaceutical and electronics firms, employing about 38 000 people. The name Research Triangle comes from the sites of three major universities—Duke, University of North Carolina, and North Carolina State University—each located about 10–15 km from the Park. There will be an excellent intellectual climate and ease in obtaining technical services. The Research Triangle Foundation, which owns the building, offered it to IUPAC in the expectation that IUPAC's presence will further enhance the stature of the Park.



Dr Edwin D. Becker, Secretary General, IUPAC

The costs of operating the Secretariat in its new location are not expected to vary significantly from those in Oxford. The extremely favourable terms for the office space will effect a considerable savings in rent, and prices for some products and services (such as computers and telecommunications) are generally lower in the United States than in Europe. Salaries are expected to be comparable or perhaps slightly higher, but significantly less in the Research Triangle area than in major metropolitan areas, such as New York and Washington. The Raleigh–Durham Airport, only a few miles from the Secretariat site, has excellent service to major American cities, daily non-stop service to London, and service through Atlanta and Washington to all world-wide destinations. With the availability of modern telecommunications, almost instant access to most countries will not be a problem.

RESEARCH TRIANGLE PARK

Although this move will entail a great deal of work on my part and that of many others, I am looking forward to reestablishing the Secretariat next year at Research Triangle Park and to taking advantage of the new locale to make the Secretariat even better than it is now. Of course, our departure from Oxford is not without regrets. IUPAC has been very happy

there, and we will unfortunately lose the services of several long-time administrative and secretarial staff members. I will have more to say about them in future columns.

A new Executive Director

It is almost impossible to imagine IUPAC without Mo Williams. Personally, I have always thought of Mo as the personification of IUPAC during the many years that I have been associated with the Union in various capacities. I am sure that many other IUPAC members have similar feelings. But Mo is looking forward to retirement at the end of April 1997. We have been advertising for a successor and seeking advice from many people inside and outside IUPAC. During the coming months the Officers will evaluate applications and, I hope, we will soon be able to report to you a successful result of our recruitment efforts.

Future scientific policy

My predecessor, Prof. Gerrit den Boef, reported to you on several occasions about the efforts being made at various levels within IUPAC to update our mission and our structure. During recent years there has been a great deal of introspective analysis within the Union of how best to manage limited resources to obtain maximum effect for chemistry world-wide. In part, this analysis has been fuelled by a number of critical assessments by Officers and by concerned scientists outside IUPAC.

This topic continues to be the central concern of the Executive Committee, as we try to insure that IUPAC will be well positioned to continue its key role in chemistry into the next century. President Fischli has taken an important step in organizing, in conjunction with UNESCO, an International Chemistry Council, composed of international leaders in academic and industrial chemistry (including four Nobel Laureates). The Council is intended to provide intellectual leadership in assessing priorities for advance in chemistry world-wide and to furnish advice on IUPAC's scientific policies. The Council is expected to operate primarily by correspondence and conference calls, rather than in plenary meetings. A charter for the Council is being prepared, and we will report further on this activity in future issues.

The Executive Committee accepted my proposal to hold short 'brainstorming' meetings to solicit advice from leaders in chemistry from industry, academia and government. We are posing the question to them: 'If you had to invent an international organization to help further the development of chemistry and the chemical industry, what would it do?' From the discussion, we hope to obtain useful ideas on updating IUPAC's mission and developing a strategic plan to guide our future development. We have organized a meeting in USA, which will have been held by the time this issue of *CI* is published, and one or more additional meetings will be planned for Europe. Results from this discussion will be available for the meeting of the Bureau in September, and I will report further to you at a later time.

The lakeside setting of the National Institute of Environmental Health Sciences in Research Triangle Park.

Meanwhile, the new Divisions of Chemistry and Human Health and of Chemistry and the Environment have been organized and are developing programs. We continue to explore other possible organizational changes that can improve our efficiency and contribute to a better understanding of the important roles that IUPAC plays in international chemistry.

Communications and publicity

Last February, with generous help from the UK's Royal Society of Chemistry, we established an IUPAC Home Page on the World Wide Web. News about IUPAC, along with a considerable amount of background information, is now available. Since this information can be updated much more rapidly than that in printed form, such as *Chemistry International*, I anticipate that the Web will increasingly become a primary means of communication to IUPAC members and to the chemistry public. The veritable explosion in the number of Web sites throughout the world and the resources now being devoted to this means of electronic communication insure that the Web will become an important part of our lives. I believe that the vast majority of IUPAC members now have or soon will have access to the Web.

Our use of the Web is only in its infancy, but we can already see its great potential for disseminating IUPAC recommendations and thus augmenting the printed versions appearing in *Pure and Applied Chemistry*. In addition, the Web should serve as a useful means for obtaining comments on Provisional Recommendations. However, there are risks in having incomplete or unapproved documents widely available and perhaps misunderstood. Our Committee on Printed and Electronic Publications has developed Guidelines for the use of the Web, which have been endorsed by the IUPAC Executive Committee. These Guidelines have been circulated to all Commission Officers and are available on our Home Page.

I urge you to visit the Home Page from time to time, and in the long run to think of ways in which this technology can be used to improve the effectiveness and visibility of IUPAC. The Universal Resource Locator code is: http://chemistry.rsc.org/rsc/iupac.htm

International Organization for Standardization

From time-to-time, *Chemistry International* publishes lists of recently published ISO standards related to chemistry. Here we profile the organization which produces these standards. An organization which has a long tradition of working to assist in the development of international standardization in many technical fields.

ISO (International Organization for Standardization) is a world-wide federation of national standards bodies, currently comprising 118 members, governed as is IUPAC by consensus. The object of the ISO is to promote the development of standardization and related activities with a view to facilitating the international exchange of goods and services, and to developing international cooperation in the spheres of intellectual, scientific, technological and economic activity. The results of ISO technical work are published as International Standards.

The scope of the ISO covers standardization in all fields except electrical and electronic engineering standards which are the responsibility of the International Electrotechnical Commission (IEC). ISO brings together the interests of producers, users (including consumers), governments and the scientific community in the preparation of International Standards.

The ISO's work is carried out through 2856 technical bodies containing more than 30 000 experts from all parts of the world. Their work has resulted in the publication of more than 10 000 ISO standards.

Origin

International standardization started in the electrotechnical field some 90 years ago. While some attempts were made in the 1930s to develop International Standards in other technical areas, it was not until the ISO was created that an international organization devoted to standardization as a whole came into existence.

Following a meeting in London in 1946, delegates from 25 countries decided to create a new international organization 'the object of which would be to facilitate the international coordination and unification of industrial standards'. The new organization, ISO, began to function officially on 23 February 1947.

Because the name of the International Organization for Standardization would have different abbreviations in different languages (IOS in English, OIN in French), it was decided to use a word derived from the Greek *isos*, meaning 'equal'. Therefore, the abbreviated form of the organization's name is always ISO.

Members

A *member body* of ISO, as with the National Adhering Organizations which constitute IUPAC, is the national body 'most representative of standardization in its country'. Member bodies are entitled to participate and exercise full voting rights on any technical committee of ISO, are eligible for Council membership and have seats in the General Assembly. By January 1996, the number of member bodies was 85.

More than 70% of the ISO member bodies are governmental institutions or organizations incorporated by public law in their respective countries. The remainder have close links with public administration in their own countries.

A *correspondent* member is normally an organization in a developing country which does not yet have its own national standards body. Correspondent members do not take an active part in the technical work, but are entitled to be kept fully informed about the work of interest to them. They may attend the General Assembly as observers. Nearly all the present correspondent members are governmental institutions. By January 1996, there were 24 correspondent members.

The ISO has recently established a third category, *subscriber membership*, for countries with particularly small economies. These subscriber members pay reduced membership fees that nevertheless allow them to maintain contact with international standardization. By January 1996, there were nine subscriber members.

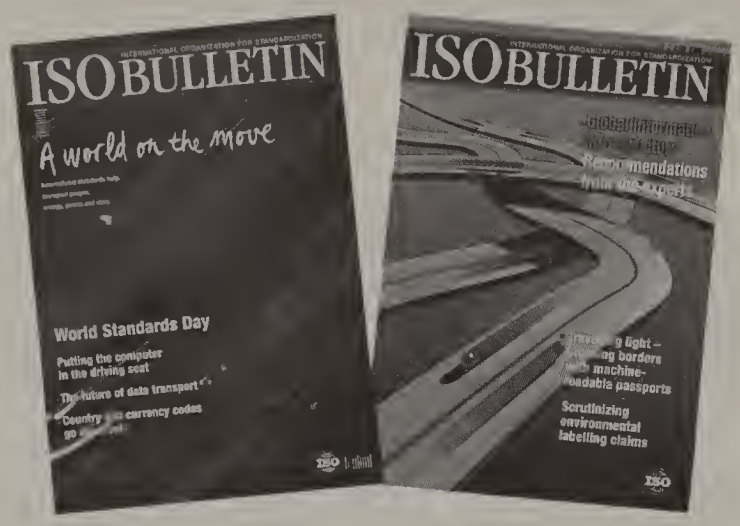
Technical work

The technical work of the ISO is carried out through technical committees. The decision to establish a new technical committee is taken by the Technical Management Board, which approves its scope. Within this area of expertise, the new committee determines its own particular programme of work.

Each technical committee may, in turn, establish subcommittees and working groups to cover different aspects of its work. Each technical committee or subcommittee has a secretariat, assigned to an ISO member body. By the end of 1995, there were 185 technical committees, 611 subcommittees, 2022 working groups and 38 *ad hoc* study groups.

A proposal to begin work in a new field of technical activity normally arises from within the ISO, but it may also originate from some other international organization. Since resources are limited, priorities must be considered. Therefore, all new proposals are submitted for consideration by the ISO member bodies. If accepted, either the new work will be referred to the appropriate existing technical committee or a new technical committee will be established. To ensure the successful coordination of work in all matters of common interest, liaisons are established between related technical committees.

Each member body interested in a subject for which a technical committee has been authorized has the right



The news magazine of the International Organization for Standardization

to be represented on that committee. Member bodies which decide to take an active part in the work of a technical committee or subcommittee are designated as participating members of that committee or subcommittee. They have an obligation to vote and, whenever possible, to attend meetings. Member bodies which wish only to be kept informed of the work of a technical committee or subcommittee are registered as observers.

How an International Standard is developed

An International Standard is the result of an agreement between the member bodies of ISO. It may be used as such, or may be implemented through incorporation into national standards of different countries.

A first important step towards the establishment of an International Standard is the committee draft. This is a document circulated for study within the appropriate technical committee or subcommittee. This document must pass through a number of stages before it can be accepted as an International Standard. Such a procedure is, by finding consensus, designed to ensure that the final result is acceptable to as many countries as possible.

When agreement is finally reached within the committee, the committee draft is sent to the Central Secretariat for registration as a Draft International Standard (DIS); the DIS is then circulated to all member bodies for voting. In many countries, the DIS is made available for public enquiry, thereby ensuring the widest possible consultations. If 75% of the votes cast are in favour of the DIS, it is accepted for further processing as a Final Draft International Standard (FDIS) which is circulated to all member bodies for formal adoption by ISO. Again, 75% of the votes cast must be in favour of the FDIS in order for the International Standard to be published. Normally, technical issues are resolved at committee level, however, the member body voting procedure provides an assurance that no important objections have been overlooked.

ISO standards are market-driven. They are developed by international consensus among experts drawn from the industrial, technical or business sectors which have expressed the need for a particular standard. These may be joined by experts from government, regulatory authorities, testing bodies, academia, consumer groups or other organizations with relevant knowledge, or which have expressed a direct interest in the standard under development.

Although ISO standards are voluntary, the fact that they are developed in response to market demand and are based on consensus among the interested parties, ensures their widespread use.

Most standards require periodic revision. Several factors combine to render a standard out of date: technological evolution, new methods and materials, new quality and safety requirements. To take account of these factors, ISO has established the general rule that all ISO standards should be reviewed at intervals of not more than 5 years. On occasion, however, it is necessary to revise a standard more frequently.

Intentional Electrotechnical Commission (IEC)

The International Electrotechnical Commission was founded in 1906. ISO and IEC have established a formal agreement, stating the relationship between these two organizations which form a specialized system for world-wide standardization. Questions related to international standardization in the electrical and electronic engineering fields are the concern of IEC. Other subject areas are the responsibility of ISO. In matters of international standardization, not related to any particular technology, ISO undertakes, in consultation with IEC, to safeguard any electrotechnical interests which may be involved. To ensure the necessary technical coordination, ISO and IEC have established a Joint Presidents' Coordination Group and a Joint Technical Advisory Board.

External relations

ISO's work is of interest to many international organizations, some of which make a direct technical contribution to the preparation of ISO standards; others, particularly the intergovernmental organizations, contribute to the implementation of ISO standards, for example by utilizing them in the framework of intergovernmental agreements. ISO has adopted arrangements for associating these organizations closely with all stages of its work:

- international organizations may make proposals for the preparation of ISO standards in a new field in the same way as ISO member bodies;
- international organizations may be granted 'liaison status' with technical committees and subcommittees. Liaison status comprises two categories: 'A' (effective contribution to the work) and 'B' (wish to be kept informed only). Liaison A gives the right to submit papers, attend meetings, and participate in discussions;
- international organizations which can make an effective contribution to the implementation of ISO

standards are expressly invited to comment on all relevant drafts; and
- technical committees are instructed to seek the full and, if possible, formal backing of the main international organizations in liaison for each ISO standard in which these organizations are interested.

Some 500 international organizations have liaison status with ISO; this includes all UN specialized agencies working in related fields. ISO has consultative status with the UN Economic and Social Council and equivalent status with nearly all other bodies and specialized agencies in the UN system.

ISO also maintains close working relations with regional groups of standards bodies. In practice, the members of such regional groups are also members of ISO and the principle is generally accepted that ISO standards are taken as the basis for whatever standards are required to meet the particular needs of a given geographical region.

Over the years, ISO has become well respected throughout the world. It has a reputation for integrity and impartiality and also enjoys a high status among international organizations (United Nations Specialized Agencies, WTO, the International Chamber of Commerce, etc.). In many sectors—such as basic mechanics, SI units, freight containers, textiles, photography and information technology, ISO standards are widely used and highly appreciated. In the 1990s the ISO name has gained increasing recognition due to the world-wide popularity and success of the ISO 9000 series.

Approaching the 21st century, ISO sees a world in which global trade between nations continues to grow at a rate 3–4 times faster than national economies; a world in which the design, manufacturing, marketing and customer service operations of a growing majority of individual enterprises are distributed across many countries; and a world in which electronic communications have dramatically increased technical collaboration between experts in academia, governments, and industries from all countries.

The increasingly rapid development of technology in many sectors will continue to present major opportunities as well as underlying dangers for the general welfare of society. It will therefore be incumbent on all social and economic partners to collaborate closely in guiding the applications of appropriate technologies toward sustainable economic development and global prosperity.

In this rapidly evolving world, globally applicable standards will play a key role. Such standards, whether developed by ISO or by others, will become primary technical instruments supporting international commerce. In this context, ISO intends to be recognized globally as an influential and innovative leader, as well as an effective and responsive producer in the development of globally applicable International Standards which meet or exceed the expectations of the community of nations. It will strive at all times to perfect the application of consensus and transparency principles in standardization, and in this way promote the values of rationality, utility, safety and environmental protection for the benefit of all peoples.

The complete documentation describing ISO's long-range strategies 1996–1998 is available from the ISO Central Secretariat:

International Organization for Standardization, 1 rue de Varembé, Case postale 56, CH-1211 Geneva 20, Switzerland. Tel.: +41 22 749 01 11; Fax: +41 22 733 34 30; E-mail: central@isocs.iso.ch and http://www.iso.ch/

PAC Review

The February 1996 issue of *Pure and Applied Chemistry* contained two sets of Plenary and Invited lectures. Firstly, there are the Plenary and Invited lectures given at the Eighth International Symposium on Novel Aromatic Compounds (ISNA-8), Braunschweig, Germany, 30 July–4 August 1995. The second set of Plenary lectures published in this issue of *PAC* were those given at the International Forum on Environmental Catalysis '95, Tokyo, Japan, 25–27 October 1995.

The Symposium on Novel Aromatic Compounds demonstrated the extraordinary versatility of organic chemists in developing new molecules and new molecular assemblies. Indeed, one can see that the modern trend in organic chemistry is not so much in synthesizing a new molecule, but in creating new architectures and complex molecular aggregates, using classical synthetic routes and self-assembly designs. Of general interest was a paper by von Ragué Schleyer & Jiao on what constitutes aromaticity.

What is aromaticity?

Paul von Ragué Schleyer and Haijun Jiao (Computer-Chemie-Centrum, Institut far Organizche Chemie Universitat Erlangen-Nurnberg Henkestrasse 42, D-91054, Erlangen, Germany).

Compounds which exhibit significantly high diamagnetic susceptibility are aromatic. Cyclic electron delocalization also may result in bond length equalization, abnormal chemical shifts and magnetic anisotropies, as well as chemical and physical properties which reflect energetic stabilization. Those compounds with high paramagnetic susceptibility may be antiaromatic.

The history of 'aromaticity', a fundamental chemical concept, began with the isolation of benzene by Michael Faraday in 1825. Many definitions or criteria for characterizing aromaticity have been considered subsequently. Some milestones are:

- before 1825: distinctive 'aromatic' smell;
- before 1865: high carbon–hydrogen ratios, that is, stable despite considerable unsaturation;
- 1865: benzene structure (Kekulé);
- 1866: substitution is more favourable than addition (Erlenmeyer);
- 1910: aromatic compounds have exalted diamagnetic susceptibilities (Pascal);
- 1925: electron sextet and heteroaromaticity (Armit–Robinson);
- 1931: theory of cyclic $(4n+2)$ π systems (Hückel);
- 1936: ring current theory—free electron circulation around the benzene ring (Pauling);
- 1937: London diamagnetism—π electron current contribution to magnetic susceptibility;
- 1956: ring currents effects on NMR chemical shifts (Pople);
- 1969: modern study of diamagnetic susceptibility exaltation (Dauben);
- 1970: magnetic susceptibility anisotropy (Flygare); and
- 1980: IGLO quantum chemical calculation of magnetic properties: chemical shifts, magnetic; susceptibilities and magnetic susceptibility anisotropies (Kutzelnigg).

These and other considerations have given rise to the following criteria of aromaticity:

1 Chemical behaviour—electrophilic aromatic substitution.
2 Structural bond length equalization due to cyclic delocalization.
3 Energetic enhanced stability (large resonance energy).
4 Magnetic 'ring current' effects:
  (a) anomalous chemical shifts,
  (b) large magnetic anisotropies, and
  (c) diamagnetic susceptibility exaltation.

Aromaticity is now associated with cyclic arrays of mobile electrons with favourable symmetries. In contrast, the unfavourable symmetry properties of antiaromatic systems lead to localized, rather than delocalized electronic structures. The 'mobile electron' arrays are not restricted to π, but may be σ or mixed in character. The latter case is illustrated by the transition states of allowed electrocyclic reactions, which were described as aromatic as early as 1938. A large diamagnetic susceptibility is the only measurable property which is uniquely associated with aromaticity. The authors discuss limitations in the other properties as sole criteria for characterizing aromatic compounds. None of these limitations are present with the 'diamagnetic susceptibility exaltations (Λ) for the same species'. Generally, Λ is defined as the difference between the bulk magnetic susceptibility (χM) of a compound and the susceptibility (χM′) estimated from an increment system for the structural components, for example, isomers without cyclic delocalization ($\Lambda = \chi M - \chi M'$).

Chemical behaviour—electrophilic aromatic substitution

Not all aromatic systems react like benzene, i.e. favour electrophilic substitution over addition. Thus, many benzenoid hydrocarbons have long been known to undergo addition reactions rather than substitution. Phenanthrene and anthracene add bromine, and the latter serves as a diene in Diels–Alder reactions. Fullerenes are aromatic, but substitution is impossible. Addition reactions are easy for C_{60}; should one conclude that it is not aromatic on this basis? Clearly, the chemical reactivity criterion is not generally applicable to many kinds of systems to which the term 'aromatic' has been applied.

Structural (geometric) criterion—bond length equalization

Bond length equalization due to cyclic delocalization is the geometric criterion of aromaticity. In aromatic hydrocarbons, the C–C bond lengths are compared with one another and with the benzene value (*c.* 0.14 nm). The direct determination of bond lengths provide valuable information on the extent of electron delocalization in molecules. In contrast, the singlet states of antiaromatic compounds are localized and generally have alternating single and double bonds which differ greatly in length, i.e. over 0.02 nm.

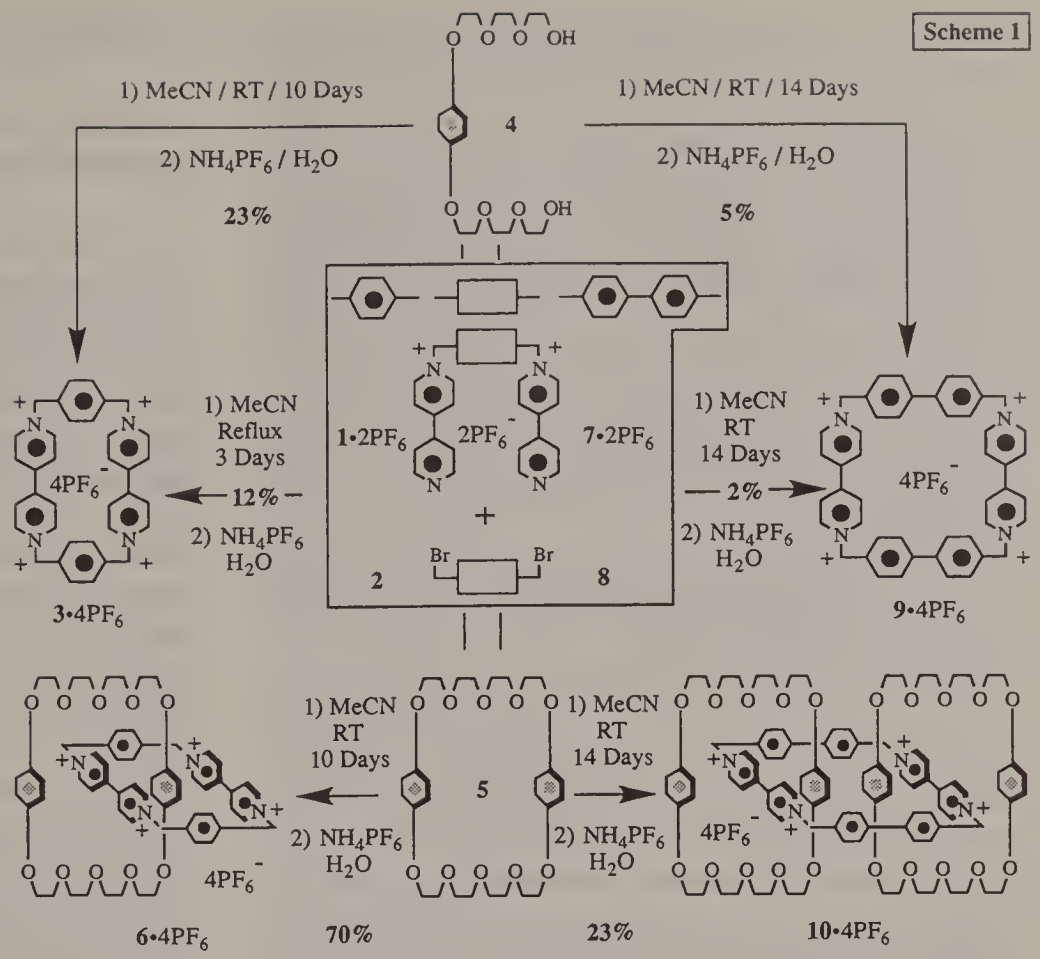
However, the geometric criterion is not generally applicable. For example, borazine, isoelectronic with benzene, has six π electrons and equalized bond lengths. But the magnetic susceptibility exaltation is only –1.7 (the benzene value is –13.4); hence borazine is not aromatic. The π electrons are largely localized on the nitrogens. Singlet cyclobutadiene and cyclopentadienyl cation are highly antiaromatic; their magnetic susceptibilities have a high paramagnetic character, +18.0 and +32.6, respectively. But the C–C bond length of the antiaromatic D_{5h} triplet cyclopentadienyl cation ground state (0.1425 nm) can hardly be differentiated from that of the aromatic D_{5h} cyclopentadienyl anion (0.1414 nm).

As an example of the type of organic chemistry which seeks to produce new assembledges of molecules, the paper by Raymo & Fraser Stoddard is a good example:

Self-assembling cyclobis(paraquat-4,4′-biphenylene)

Françisco M. Raymo & J. Fraser Stoddart (School of Chemistry, University of Birmingham, Edgbaston, Birmingham, B15 2TT, UK).

The template-directed syntheses of the bipyridinium-based cyclophanes cyclobis(paraquat-*p*-phenylene) and cyclobis(paraquat-4,4′-biphenylene) can be achieved by employing π-electron rich hydroquinone-based and ferrocene-based templates. By employing macrocyclic hydroquinone-based polyether templates, [2]catenanes and [3]catenanes, in which the bipyridinium-based cyclophane is mechanically interlocked with the macrocyclic template(s), can be self-assembled in solution. The introduction of ester functions within these polyether chains of the macrocyclic templates provides



Hydroquinone-based guests as templates.

the possibility of degrading the catenated structure via ester hydrolysis, thus releasing the tetracationic cyclophane originally trapped within the catenane. The use of ferrocene-based templates provides a more efficient way to synthesize the bipyridinium-based cyclophane incorporating bitolyl spacers. In particular, the use of a 1,1′-disubstituted polyether ferrocene derivative provides the possibility of obtaining the tetracationic cyclophane, cyclobis(paraquat-4,4′-biphenylene)—accessible only in very low yields, without the use of a template—on a preparative scale.

Self-assembly processes are based upon the attainment of high complementarity between simple modular components which serve as subunits. Weak noncovalent bonding interactions bring the subunits together, affording an initial superstructure in a so-called nucleation step. By a series of cooperative noncovalent bonding interactions, the initial superstructure evolves into the final thermodynamically stable supramolecular architecture which can be captured by the formation of covalent bonds, sometimes in kinetically controlled processes. Remarkable efficiency overall, a high degree of control, and error checking and recovery are ensured throughout the process. These features suggest the use of self-assembly processes as a viable alternative to the traditional synthetic methodologies for the generation of wholly synthetic systems that are rather intricate. Recently, we have developed a synthetic approach to the self-assembly of interlocked molecular compounds, such as catenanes and rotaxanes, as well as supramolecular arrays such as pseudorotaxanes. The methodology relies upon the complementarity that exists between π-electron deficient bipyridinium-based macrocyclic components and π-electron rich hydroquinone-based acyclic and cyclic polyethers. In their early stages, self-assembly processes are driven by noncovalent bonding interactions such as (i) π–π stacking between the π-electron deficient bipyridinium units and the π-electron rich hydroquinone residues, (ii) hydrogen bonding between the polyether oxygen atoms and the hydrogen atoms in the α-positions with respect to the nitrogen atoms of the bipyridinium units, as well as (iii) edge-to-face T-type interactions between the hydrogen atoms of the hydroquinone residues and the π-clouds of the aromatic spacers incorporated within the tetracationic cyclophanes. The template-directed synthesis of cyclobis(paraquat-4,4′-biphenylene)—a molecular square—has been achieved by self-assembling the bipyridinium-based cyclophane—the host at the end of the process—around preformed π-electron rich component(s)—the guest in the beginning.

International Forum on Environmental Catalysis '95, Tokyo, Japan, 25–27 October 1995

There were three invited talks, and a summary of the contents of these talks is given below.

Catalytic science and technology for environmental issues

K. I. Zamaraev (Boreskov Institute of Catalysis, Novosibirsk, Russia)

In the first part of this lecture it was demonstrated how knowledge that comes from studies of catalysis at the molecular level helps to design new, more efficient catalysts and catalytic processes. In the second part the importance of catalytic technologies for solving environ-

mental issues and providing sustainable development was discussed. It was demonstrated how catalysis helps to protect the ozone layer, to combat the greenhouse effect, to create environmentally safer transport, to solve environmental problems of energy production, to prevent pollution by H_2S in gas and oil mining and by CH_4 in coal mining, to purify exhausts of chemical and various other industries, to provide the highest energy efficiency and minimize consumption of raw materials in the chemical, petroleum and other industries, to process renewable raw materials, such as biomass, into valuable chemicals. In the third part, the role of the natural abiotic catalysis in the chemistry of the troposphere was discussed.

Catalysis is the backbone of the chemical industry. It is also a fundamental feature of all life processes and of chemistry of the environment.

In the past three decades we have witnessed in the scientific study of catalysis a continuous shift from phenomenological approaches to structural and mechanistic investigations at the molecular level. The engineering of catalytic reactors has also become more strongly based on a deeper understanding of reaction mechanisms, mass- and heat-transfer phenomena in catalyst pores, pellets and beds, and the mathematical modelling of catalytic processes.

Dimethyl carbonate for environmentally benign reactions

Yoshio Ono (Department of Chemical Engineering, Tokyo Institute of Technology, Ookayama, Meguro-ku, Tokyo, 152 Japan)

The chemical industry has been one of the major economic activities of this century and will also be so in the coming century. However, the industry has been blamed for producing environmentally hazardous substances, which cause acid rain, a reduction of stratospheric ozone levels and so on. Therefore, many efforts have been focused on eliminating or decreasing environmentally hazardous substances. In fact, the industry as a whole reduced its emissions to air, land, and water by 41% between 1987 and 1991, while overall production increased by more than 10%. Thus, NO and SO are one of the major targets in this respect. Fluorocarbons and perchlorinated benzene are other examples.

Dimethyl carbonate (DMC) is a unique molecule, having a versatile reactivity. The transesterification of DMC with phenol gives methyl phenyl carbonate, which is converted into diphenyl carbonate (DPC) by disproportionation. MoO_3/SiO_2 is an active catalyst for both reactions. DPC is an essential monomer in the non-phosgene route for polycarbonates. The methoxycarbonylation of aniline gives methyl N-phenyl carbamate in the presence of a lead compound. This reaction offers a non-phosgene route to isocyanates.

As a methylating agent, DMC can be a substitute for methyl halides and dimethyl sulfate, toxic and corrosive chemicals. Phenylacetylene, aniline and phenol are selectively methylated with DMC over zeolites in the vapour-phase. The reaction of DMC with silica offers a simple and clean method for synthesizing $Si(OCH_3)_4$.

Low NO_x options in catalytic combustion and emission control

R. Burch (Reading Catalysis Centre, Department of Chemistry, The University of Reading, Whiteknights, Reading, Berkshire, RG6 6AD, UK)

The options for preventing the release of nitrogen oxides into the atmosphere from combustion processes was considered, both from the viewpoint of using catalytic combustion to prevent the formation of nitrogen oxides, and of using hydrocarbons for the selective reduction of nitrogen oxides to nitrogen in the presence of excess oxygen. The combustion of methane at low temperatures on palladium-based catalysts was discussed, and some new results relating to the nature of the active catalyst and the rate-determining step were presented.

Current attempts to develop selective reduction catalysts for the removal of nitrogen oxides were summarized and the particular advantages and disadvantages of platinum group metal-based catalysts were discussed. The mechanism of the nitrogen oxide to nitrogen reaction is considered and some new results were presented which are consistent with a dissociative mechanism, possibly involving adsorbate-assisted dissociative adsorption of nitric oxide.

Nitrogen oxides (NO_x) are serious pollutants, and legislation requires that the emission of NO_x is strictly limited. Most combustion processes result in the formation of NO_x, which may arise either from fuel-bound nitrogen or by nitrogen fixation in high temperature flames. It is difficult to prevent the formation of NO_x from fuel-bound nitrogen so that 'end-of-pipe' methods must be utilized to eliminate the pollution. Ammonia is well established as a selective reductant for NO_x in large scale stationary applications, and Pt/Rh-based catalysts are widely used in mobile sources, such as gasoline engines operating close to the stoichiometric air/fuel ratio. Nitrogen fixation, on the other hand, can in principle be prevented by improving the control of the temperature in a flame, since the reaction of N_2 only occurs at a significant rate at temperatures well above the *average* flame temperature. To some extent this can be achieved by a redesign of the burner system, but for very low levels of NO_x emission, catalytic combustion may provide an acceptable solution. In situations where catalytic combustion is not possible or not economic, alternative strategies must be adopted. Recently, there has been much interest in developing catalysts which will be selective for the reduction of NO_x in the presence of a large excess of O_2 (lean-burn conditions) where the reductant is a *hydrocarbon* rather than ammonia. A number of different systems have been studied, ranging from nonreducible oxides and zeolites, through base metal redox systems, to supported platinum group metals. In his paper the author considered some fundamental aspects of the platinum group metal catalysts used for catalytic combustion and for the selective reduction of NO_x with hydrocarbons.

Summary Minutes from the meeting of the IUPAC Commission on Thermodynamics (I.2) at the IUPAC General Assembly in Guildford, 5–6 August 1995

Seventeen members of the commission met to review progress since the meeting at Clermond-Ferrand, France, in the summer of 1994.

Ongoing projects

(i) The Electrolyte Solution Data project saw two volumes published, a third to appear in late 1995, a fourth in preparation, and the submission of Chapter 17 to the IUPAC book *Theory of Equations of State for Fluids and Fluid Mixtures*. (ii) The second phase of the horizontal project *Advanced Materials* has been completed, with the publication of three papers in *Pure Appl. Chem.* 1995, **67**, 919–930, 931–935, 939–946. (iii) Recommendations for phase diagram nomenclature were approved for discussion with the Chairs of the other Commissions. (iv) The progress report for the IUPAC text in (i) above indicated that 10 of the 19 chapters were complete. (v) The Teacher's Version of *Standard Quantities in Chemical Thermodynamics* was published in *J. Chem. Thermodyn.* 1995, **27**, 1–16. (vi) Two major projects were completed for the Thermodynamic Data project, a third is in press and significant progress was made on four others, with publication of part of these results. Two new projects were investigated, one of which was approved for formal initiation procedures. (vii) Results form the Transport Properties work were published in *Int. J. Thermophys.* 1994, **15**(1), 1; **15**(4), 647; **15** (5), 767. Another project is near to completion with the text *Transport Properties of Fluids* (Cambridge), to appear in 1996. (viii) Results from the project *Thermodynamics of Enzyme-Catalysed Reactions* have been published in *J. Phys. Chem. Ref. Data* 1994, **23**, 1035–1103, and two others are in press.

New projects

Commission approval was given for: (i) project initiation *Thermodynamics of Chemical Reactions: Nomenclature & Symbols*, and (ii) feasibility study for the preparation of a new edition of *Experimental Thermodynamics* Vol. II, and (iii) submission for IUPAC approval of the *Guidelines for Publications of Equations of State*.

Joint meetings

(i) *Steering Committee on Biophysical Chemistry*: The current status of the study on recommendations for Measurement and Presentation of Results by DSC were outlined. It was agreed that the project on Thermodynamics of Enzyme-Catalysed Reactions should proceed to the next stage and that, with the creation of the new Biophysical Chemistry Commission, these projects should go forward through IUPAC as joint projects with the I.2 Commission.

(ii) *I.3 Electrochemistry Commission*: Phase 1 of the work on Redox Potentials of Proteins was reviewed and an appeal made for assistance from I.2 Commission members. Discussions re nomenclature for the chemical potential indicated no possibiity in the near future of standardizing the symbolism used in electrochemisty and in the main stream of thermodynamics.

(iii) *I.2 Subcommittee on Thermodynamic Data*: Extensions were approved for five projects to allow publication of results.

(iv) *I.2 Subcommittee on Transport Properties*: Three projects were approved.

(v) *I.2 Subcommittee on Chemical Data Bases*.

Other business

The Commission agreed to start proceedings with the International Organization for Standardization and Commission I.2 to have the equilibrium constant K without a superscript designated as the only internationally accepted symbol.

The next meeting will be held at the 12th Internatinal Conference on Chemical Thermodynamics, Osaka, Japan, 25–30 August 1996.

Prof. Ron D. Weir
(Secretary of Commission I.2)

Subcommittee I.2 on Thermodynamic Data

Excellent progress was reported in all the Subcommittee's current projects:

Activities of the IUPAC Thermodynamic Tables Project Centre

The new methane volume of the *International Thermodynamic Tables of the Fluid State* is now available in draft form and has been circulated in draft form prior to publication. It will become volume 13 in this series.

The work on benzene is proceeding with high priority. A new representation of the two-phase region has been finished.

It has become feasible to resume work on sulphur hexafluoride, which had been suspended because of conflicting experimental data sets. New data has now become available that will help remove the contradictions.

Critical compilations

The *Critical Compilation of Vapour–Liquid Critical Properties* (introduction and survey of experimental methods, alkanes, and aromatic hydrocarbons) have been published in the *Journal of Chemical Engineering Data*.

Part 4 (alcohols) is in press. Work of the other parts of this series is continuing according to schedule.

The data collection: *Activity Coefficients at Infinite Dilution in Nonelectrolyte Mixtures: A Critical Compilation* now contains more than 500 references, over 1300 individual substances and 1200 solute-solvent pairs, and more than 36 000 γ^{∞} values. Critical evaluation of this data is proceeding.

Workshops on properties of binary and ternary mixtures of ethers and alkanes and alcohols

A part of session 2 (nonelectrolytes) of the 13th IUPAC Conference on Chemical Thermodynamics, Clermont-Ferrand (1994) was devoted to this topic. Selected papers will appear in a special issue of *Fluid Phase Equilibria*.

Related projects

The *Guidelines for Publications of Equations of State* had originally been started as a Subcommittee project, but has been taken over by Commission I.2. Because it constitutes a set of recommendations, draft copies were sent to several referees. Minor changes are being made prior to publication.

Volumes on dielectric properties of water and aqueous solutions as well as higher alkanols have been published in the *DECHEMA Chemical Data Series: Electrolyte Data Collection*. A volume on nitriles is in print.

Prof. Ulrich K. Deiters
(Secretary of Subcommittee I.2)

Summary minutes of the meetings of the Commission on Physical Organic Chemistry (III.2), Guildford, 5–7 August 1995

During its meetings in Guildford, August 1995, the Commission paid a great deal of attention to the future of physical organic chemistry. It was decided to propose to the Division a project called 'Physical Organic Chemistry in the 21st Century'. It was anticipated that the major result of this project will consist of a collection of approximately 20 essays of 5–10 pages in length from respected chemists drawn from various areas. A feasibility study for such a project is almost completed and the proposal has been submitted. This rapid pace is in line with recommendations that IUPAC needs to complete its work more expeditiously. Reactions from a number of experts were, in general, highly favourable.

Commission of Physical Organic Chemistry. Standing from left to right: Y.Takeuchi, D.J. Raber, J.-L.M. Abboud, W. Drenth, T.T. Tidwell, O. Tarhan, S.S. Kim, C.L. Perrin, E. Humeres and S. Fukuzuni. Sitting from left to right: C.J.M. Stirling, H.-U. Siehl, Z. Rappoport, V.I. Minkin, J.R. Zdysiewicza and J. Shorter.

Progress reports on the ongoing projects were presented and approved. All these projects are expected to be completed after a period of 4–5 years. Several projects are concerned with computational chemistry. Liaison exists with the Working Party on Theoretical and Computational Chemistry in the Division of Physical Chemistry.

Being aware of its responsibility to mankind, the Commission intends to play a role in the solution of environmental problems. Appropriate projects will be formulated.

To improve and to speed up the dissemination of its project reports and to facilitate interaction with the chemistry community at large, the Commission is urging IUPAC to go on the Internet and the Commission intends to be a leader in the use of this medium. Moreover, IUPAC is commended for its move to accept material on disks, but is advised to do this in a user friendly way and to provide not only for PC but also for Apple computers. The Commission noted with pride that a distinguished physical organic chemist (Professor George A. Olah) had been awarded the 1994 Noble Prize in Chemistry.

The next series of meetings will be held in Seoul, Korea, probably after the International Conference on Physical Organic Chemistry which will take place over 25–29 August 1996.

Prof. Tom T. Tidwell (Chair) and Prof. Wiendelt Drenth (Sec.)
(Commission III.2)

Summary minutes of meetings of Commission III-3 (Photochemistry) at the 38th IUPAC General Assembly, Guilford, 4–11 August 1995

Eight members of the Commission attended the 38th IUPAC General Assembly. Five meeting sessions were devoted to work on the current projects, the definition of new projects, changes in the membership of the commission, exchanges with other Commissions, and discussions on desirable changes in the way that IUPAC Divisions and Commissions operate.

Current projects

The final version of the 'Glossary of Terms used in Photochemistry (2nd edn) including Terms used in Photoinduced Electron Transfer', taking into account the comments received from the IDCNS and various international sources, will be written by Prof. I. Verhoeven, coordinator of the project but no longer a member of the Commission.

After revisions and additions suggested by the Com-

mission during the discussions at Guilford, the documents on 'Methods for the Evaluation of Transient Absorption Kinetic Data' and on 'Figures of Merit for the Technical Development and Application of Advanced Oxidation Processes' (first part of the project on 'Water Treatment and Photocatalysis') should be very close to their final version but should be examined by external experts before being submitted for publication.

Major modifications and revision of the document on 'Quantum Yields and Turnover Numbers in Heterogeneous Photocatalysis' were requested by the Commission. This second part of the project on 'Water Treatment and Photocatalysis' will therefore be separated from the first to avoid undesirable delay in the publication of the 'Figures of Merit...'. One new Associate Member, Prof. Pelizzetti, and the new Chairman, Prof. Bolton, will assist the assist the author (N. Serpone, not a Commission's member) in this task.

New or future projects

Our Chairman maintained contacts with Prof. H.H.Tønnesen from the Institute of Pharmacy at the University of Oslo, but the proposal that our Commission should provide expertise in the definition of the procedures for testing the 'Photostability of Drugs' found very little echo in the pharmaceutic community. Prof.Tønnesen recently wrote that, in her opinion, 'there is no present need for an IUPAC project in the area of photostability testing of drugs'.

Dr E. Vrachnou-Dorier specified the content of a possible project on 'Photochemical Solar Energy Conversion and Storage'. She proposes the creation of a database accessible via the Internet and including known data on the reactions and the reactants whoch are (potentially) useful for the photochemical conversion and storage of solar energy. This project faces a major problem—financial cost—but its feasibility will be studied by Dr E. Vrachnou-Dorier who becomes an Associate Member of the Commission.

Another new Associate Member, Dr Acuna Fernandez, was asked to define the content and limits of a future project on the problems arising from light polarization in studies of films of biological or polymeric macromolecular systems. Commission I-6 (Colloid and Surface Chemistry including Catalysis), is interested in such a project and should be informed of any development of this idea.

Prof. J. Bolton's suggestion that a combined volume should be published of all the Commission's documents finalised to date should be pursued; certainly, for many photochemists, this would greatly facilitate access to these documents and would increase the impact of the Commission's work on the photochemical community.

Changes in the Commission's membership (effective in January 1996)

The titular member position of Prof. F. Scandola, who resigned his membership, was attributed to Prof. J. Bolton, elected as new Chairman. Four new associate membersjoined the Commission: Dr U. Acuna Fernandez, Prof. H. Bouas-Laurent, Prof. E. Pelizzetti and Dr E. Vrachnou-Dorier. New National Representatives, proposed by their National Organizations, were accepted by the Commission: Dr V. Toscano (Brazil), Dr B. Pandey (India) and Prof. S. Içli (Turkey).

R. Bonneau
(Commission III.3)

Summary minutes of meetings of the Commission on Separation Methods in Analytical Chemistry (V.3), Guildford, 5–7 August 1995

The meeting of the Commission during the IUPAC General Assembly in Guildford was well attended, with members coming from India, Russia, Slovakia, Spain, Greece and Sweden, as well as the UK. They were welcomed by the Commission Chairman, Dr Aurel Marton from Hungary.

Although no new papers had been published in the last year, two nomenclature proposals on nonlinear chromatography by Dr Jan-Ake Jonsson and on chiral chromatography by Prof. Vadim Davankov were available for public review. Following discussion at the meeting, a paper on liquid chromatographic stationary phases from Prof Roger Smith was completed and will shortly be submitted for review. A further paper on a method for the characterization of ion-exchange materials was close to completion. Discussions at the Commission led to two new projects being initiated, the first on liquid chromatographic liquid phases. The second new topic is the important new area of capillary electrophoretic methods, where co-ordination is needed to systematise an 'alphabet soup' of new terms, which are arising from different parts of the world and as workers move into the field from different backgrounds. Much of the meeting looked forward to possible future projects. It considered not only chromatographic methods, but also other separation techniques employed by analytical chemists. It was also recognized that many future projects may need to be undertaken in collaboration with other Commissions and that their instrumentation (e.g. spectrometers) are often the detectors in chromatographic separation. Alternatively the separation methods of interest to the Commission are the tools to carry out applications in such fields as polymer characterization, environmental analysis or speciation studies.

A spin-off from an earlier project on the 'Nomenclature for Chromatography' excited considerable interest both in the Commission and in the Division. It had recently it had been developed by a chemical company as a Windows help file, meaning that it could be accessed and searched on virtually any PC. The company hoped to make it freely available as part of a computer-readable product catalogue which could reach many thousands of chromatographers. The possibility of expanding this information technology approach to

make published papers freely available from the Commission via the Internet will be explored in the future. This led to a more general debate on the potential for publicising the activities of IUPAC. It was noted that papers alerting the chromatographic community to the work of the Commission had appeared in a number of publications, many of which would receive a much wider readership than the *Pure and Applied Chemistry*. The Commission had also used poster displays at international symposia to promote its work and the Nomenclatures for Chromatography.

An increase in the membership to four titular members was welcomed, although the Commission was still the smallest in the Division. However, this would now provide the potential to develop further projects and to expand the scope of the Commission's work. The Secretary, Prof. Roger Smith, also apologised to the members of the Commission for the conversion of Analytical to Analytic in the last summary minutes to appear in *Chemistry International*. He assured them that had been a gremlin in the Editorial Office rather then a renaming of the Commission or the Division. Finally the members of the Commission were pleased to accept an invitation from Prof. Panos Siskos to host their next meeting in Athens in 1996.

The next meeting of the Commission will be held in Athens, Greece, in late August 1996.

Prof. Roger M. Smith
(Secretary of Commission V.3)

Summary minutes from the meeting of the IUPAC Commission on Soil and water Chemistry (VI.3) at the IUPAC General Assembly in Guildford, 5–7 August 1995

The major topics discussed during this meeting were the restructuring of the Applied Chemistry Division and its implications for the Commission on Soil and Water Chemistry, the new composition of the Commission, and the progress of current projects. Thereupon, meetings with other Commissions were arranged to discuss co-operation on several topics.

With much appreciation from the Commission on Soil and Water Chemistry for the work that he has been doing over the past 10 years, Dr Dobbs decided to resign as Chairman of the Commission. At Guildford, the Applied Chemistry Division approved the proposal made by the Soil and Water Chemistry Commission to appoint Dr Y. Shevah as the new chairman for the period 1996–1997.

Since the last meeting of the Commission (Italy, 1994), two contributions to *Pure and Applied Chemistry* have been published. A report of the Workshop on Quantitative Structure Biodegradability Relationships was also completed in the last year. Thereupon, a first draft manuscript was prepared for circulation among Commission Members and other IUPAC Commissions involved, on the importance of natural organic material for environmental processes in waters and soils. Several ideas for new projects were discussed and it was decided that a workshop on factors influencing the transport of pollutants in soil systems will be organized next year.

Before discussing the progress of current projects and before initiating new projects, attention was paid to identify those areas to which the Commission on Soil and Water Chemistry can contribute in the near future. The following areas were indicated as being of major interest:

1 Disinfection and disinfection products from water treatment.
2 Interactions between water, biofilm and pipe materials of microbiological processes in water distribution systems and the role of microfiltration/ultrafiltration membranes in drinking water treatment plants. A working party on microfiltration/membrane techniques will be established.
3 Pesticides in soil and water. In this area, joint action with the Agrochemicals Commission will be undertaken.
4 Testing of poorly soluble chemicals.
5 Oestrogenic chemicals in the environment.

Feasibility studies will be initiated in all areas indicated, in addition to the following feasibility studies: 'Variability in commercial standards for water analysis', 'Statistical performance standards of analytical methods for soil and water analysis', 'Control of remediated soil', 'Quality standards for soil and water', 'The occurrence of Arsenic in drinking water' (joint project with Commission VI.1).

Within the next 2 years the following projects will be completed by Commission VI.3: 'Importance of Natural Organic Material for Environmental Processes in Waters and Soils' (draft paper available), 'Quality of Chemical Data in Databases', 'Code of Practice for Reporting Analytical Data for Environmental Samples', 'Environmental fate of organic micropollutants in international rivers', 'Measurement of chlorine residuals in water', 'Trends in nonconventional supply of water (water-reuse) and their environmental effects', 'Water treatment using membrane separation processes', 'The chemical properties of sewage sludge', 'Solute movement in soils with potential rapid by-pass movement', 'Modelling lifetime and degradability of organic compounds in soil and water systems'.

In either September or October 1996, a workshop will be organized, entitled: 'Environmental transport of pollutants—the influence of natural organics and soil structure'. In this workshop the results of the projects on natural organics and solute movement will be presented.

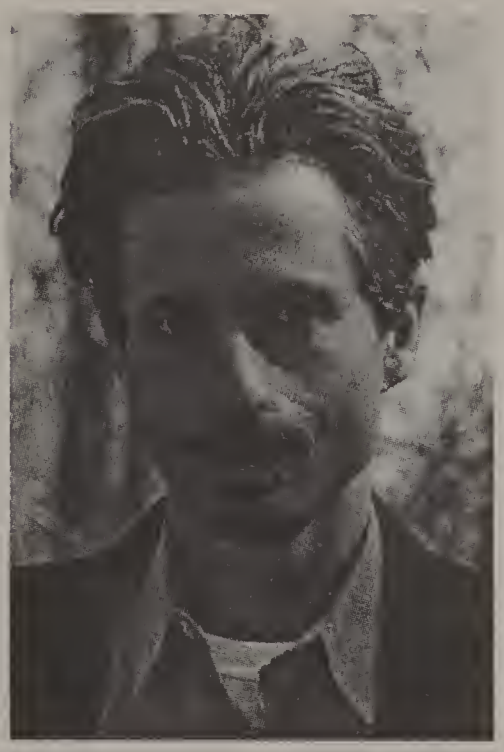
The next meeting will be held at the Fraunhofer Institute (Schmallenberg, Germany) and will coincide with the workshop 'Environmental transport of pollutants—the influence of natural organics and soil structure' (September or October 1996).

Dr Willie Peijnenburg
(Secretary of Commission VI.3)

The Thieme–IUPAC Prize

Georg Thieme Verlag, the International Union of Pure and Applied Chemistry and the Editors of Synthesis, Synlett and Houben-Weyl are pleased to announce the recipient of the Thieme–IUPAC Prize in Synthetic Organic Chemistry 1996

Eric N. Jacobsen



The Thieme–IUPAC Prize, consisting of DM 10 000, is awarded every 2 years on the occasion of the IUPAC International Conference on Organic Synthesis (ICOS) to a scientist under 40 years of age, whose research has had a major impact on the field of synthetic organic chemistry. The third Thieme–IUPAC Prize was presented at an Award Talk on 2 July 1996 at the ICOS-II in Amsterdam, the Netherlands.

Eric Jacobsen was born on 22 February 1960 in Manhattan, USA. He was raised in New York City, and he obtained his BS degree from New York University in 1982. As an undergraduate, he carried out research in the laboratories of Yorke E. Rhodes. His PhD work was done at the University of California, Berkeley, in the field of organometallic chemistry under the direction of Robert G. Bergman. In 1986, he returned to the East Coast for a National Institute of Health postdoctoral fellowship at the Massachusetts Institute of Technology with K. Barry Sharpless, where he was one of the initiators of the asymmetric catalytic dihydroxylation project. In 1988, he took on a faculty position at the University of Illinois at Urbana-Champaign where he was promoted to associate professor in 1991. He moved to Harvard University as full professor in the summer of 1993, and he currently directs a research group of 20 graduate students and postdoctorates at Harvard. He is also a consultant at Merck, Sepracor and Versicor.

Eric Jacobsen has emerged as the best young chemist in the world working at the important frontier of designing/discovering selective catalysts for use in organic synthesis. He began his career at Illinois in spectacular fashion with his new process for the asymmetric epoxidation of unfunctionalized olefins. This was a major accomplishment for both conceptual reasons and, especially, for practical applications in synthesis. The Jacobsen catalyst, which was Fluka's reagent of the year in 1994, is a chiral, catalytically active transition metal complex. The reagent has allowed an easy access to a number of enantiomerically pure epoxides. A number of them have allowed the expeditious synthesis of pharmacologically active products. One such example is the synthesis of the taxol side chain.

In Eric Jacobsen's brief time at Harvard, he has continued to be extremely productive in the area of asymmetric catalysis. This time, he has found a practical catalytic system for highly enantioselective ring openings of epoxides and aziridines. As with the Jacobsen epoxidation, this new process is so simple and efficient that it is essentially ready for immediate industrial application. A recent synthetic example is the synthesis of a prostaglandin chiral building block. This asymmetric catalytic method represents an attractive alternative to enzyme-based procedures.

Eric Jacobsen is widely regarded as a most dedicated researcher and a fearless experimentalist. He is already perceived as a clear leader in the field of asymmetric catalysis, and we can expect many more exciting developments from his laboratories in the discovery and mechanistic elucidation of new reactions of practical value.

Eric Jacobsen has been the recipient of numerous awards including the NSF Presidential Young Investigator Award, the Packard Fellowship, the Camille and Henry Dreyfus Teacher-Scholar Award, the Alfred P. Sloan Foundation Fellowship, the Cope Scholar Award, and the Fluka Prize.

Erratum

The last issue of *Chemistry International* contained an incorrect caption for the picture of the finance committee (p. 175). It should have read:

Finance Committe meeting in Zurich; left to right: Dr M.M.G. Senden, Prof. E.J. Grzywa, Prof. John Ward (IUPAC Treasurer and Chairman) and Dr E.P. Przybylowicz, with Dr Mo Williams (Secretary) standing.

News

New commission formed on biophysical chemistry

The formation of a new commission (Commission I.7, on Biophysical Chemistry) in the Physical Chemistry Division was approved at the meeting of the Council in Guildford, UK, at the last General Assembly, August, 1995, and was established 1 January, 1996. The Terms of Reference of this new Commission are:

1 To alert the scientific community to the application of physicochemical methods to biological problems.
2 To highlight areas related to biophysical chemistry where there is confusion regarding definitions, nomenclature, symbols and related matters, and to establish guidelines and recommendations.
3 To establish contacts with other IUPAC bodies with the aim of initiating interdisciplinary joint projects related to biophysical chemistry.
4 To promote communications between the Physical Chemistry Division and other bodies dealing with biology such as IUPAB and IUBMB that deal with biophysics, biochemistry and molecular biology.
5 To contribute to future IUPAC activities in biologically related areas.

There are currently three Titular Members: Prof. H. Hauser, Chairman (Switzerland), Dr R. N. Goldberg, Secretary (USA) and Prof. K. W. Würthrich (Switzerland) and 9 Associate Members: Prof. M. Caffrey (USA), Dr A. Cornish-Bowden (France), Prof. D. Eisenberg (USA), Prof. W. VanGunsteren (Switzerland), Prof. T. Kitagawa (Japan), Prof. W. Saenger (Germany), Dr T. R. Stouch (USA), Prof. D. R. Th'evenot (France) and Prof. A. Wada (Japan).

Presently, there are three short-term Titular Members on closely related projects. These are Prof. F. M. Hawkridge (USA), Prof. H.-J. Hinz (Germany) and Dr F. P. Schwartz (USA). The projects currently being undertaken with this new Commission are: Electrochemical Biosensors; Terminology in the Field of Lipid Vesicles (Liposomes): Preparation and Essential Characterization; Standardization of Data Bases on Protein Structures Determined by NMR in Solution; A Nomenclature of Lipid Mesophases; Recommendations for the Measurement and for the Presentation of Results Obtained on Biological Substances with Scanning Calorimetry; and Thermodynamics of Enzyme Catalysed Reactions.

Nitric oxide (NO): a surprising biological regulator

Research papers continue to appear with new insights into the biological activity and potential clinical uses of nitric oxide (NO). Each new publication adds to nitric oxide's already lengthy list of functions in controlling the circulation of the blood, and regulating activities of the brain, lungs, liver, kidneys, stomach, gut, genitals and other organs. The molecule governs blood pressure, through a recently recognized process that contradicts textbook wisdom. The immune system uses nitric oxide in fighting viral, bacterial and parasitic infections, and tumours. Nitric oxide transmits messages between nerve cells and is associated with the processes of learning, memory, sleeping, feeling pain, and, probably, depression. It is a mediator in inflammation and rheumatism.

Five years ago, the Wellcome Institute for the History of Medicine began a series of 'Witness Seminars' to provide a forum for recording first-hand accounts of the circumstances leading to major advances in contemporary biomedical science. It is hoped that such seminars will capture the sort of reminiscences, and perspectives, that come only from the intimacy of an autobiography of those in the front-line of the research.

One such opportunity to savour a first-hand narrative of an area of research in the making was provided last year by Prof. Salvador Moncada (University College London, UK), Dr Patrick Vallance (University College London, UK), Prof. John Garthwaite (Glaxo Wellcome plc, Beckenham, UK) and Prof. Eddy Liew (University of Glasgow, UK). They distilled the significance of a welter of basic and clinical research by scores of international laboratories, into how nitric oxide, synthesized from the amino acid L-arginine, found in cells from head to foot, can keep us fit and healthy.

Research on the biological impact of NO is now yielding thousands of publications a year. The story began with the discovery that the nitric oxide molecule was the regulator of the muscle tone of blood vessels. While this finding astonished some scientists and provoked scepticism in others, it opened a floodgate of additional publications. The potential importance of this research, which showed that nitric oxide governed numerous other biological processes, received an accolade guaranteeing public attention when nitric oxide was chosen as the cover story by the editors of *Science* for its 'Molecule of the Year' issue in 1992, and was wreathed with puns: NO sex; NO wonder; NO way.

Salvador Moncada was a senior author of the paper published in 1987 which revealed how nitric oxide is produced to control the relaxation of the muscles of blood vessels. He recalls the surprise expressed by other researchers when they realised that such a crucial activity—with profound implications for understanding cardiovascular diseases—was under the control of such an apparently simple molecule.

It had previously been established that blood vessels, nurtured in an organ bath, relaxed when chemically stimulated. If the inner layer of cells of an artery or vein

(the endothelium) was absent, the smooth muscles of the blood vessel lost their capacity to make the vessel expand. This showed that a previously unrecognized substance must exist to regulate the tone of the smooth muscles of blood vessels. They referred to the mystery agent as endothelium dependent relaxing factor (EDRF). Curiosity provoked several laboratories to start searching among the body's complex biomolecules to find a candidate for EDRF among the array of amines, peptides, fatty acids and other chemicals.

Salvador Moncada and his colleagues devised two experiments to test whether nitric oxide could account for the actions of EDRF. The first was to determine whether nitric oxide was released by endothelial cells. Equipment developed for the study included a highly sensitive, miniaturized version of an instrument used in the car industry to measure nitric oxide in the exhaust of petrol engines. When linked to endothelial cells, repeated measurements demonstrated that nitric oxide was indeed the relaxing factor released by these cells. The second experiment compared the effects of natural EDRF on muscle tone with the effects produced by mimicking the relaxing factor with nitric oxide purchased from a standard chemical supplier.

Salvador Moncada recalled that nobody had the remotest suspicion that EDRF would turn out to be as simple a molecule as nitric oxide; or that it was synthesized not just in the blood vessels, but as an essential part of the physiology of most organs and tissues.

Previously, nitric oxide was regarded as an environmental pollutant—at best a chemically reactive nuisance, at worst a poison. In the exhaust fumes of cars it reacted readily with oxygen to produce smog, increasing the risk of asthma. When discharged into the atmosphere from power station chimneys it contributed to ecological damage from acid rain. Consequently, a response bordering on disbelief greeted the discovery that cells lining the walls of blood vessels—endothelial cells—intentionally synthesized nitric oxide as a muscle relaxant. Nitric oxide is short-lived when in contact with other molecules, and a constant supply is generated by endothelial cells in response to the sheer stress of the blood flow on the artery wall. The notion that such a molecule—normally considered a poison or a pollutant—should also hold a key to a healthy body and mind was counter-intuitive, and is still disconcerting to some people.

A year after identifying nitric oxide as the mystery molecule, Salvador Moncadat's group reported on how it was formed in endothelial cells. Its biochemistry depends on the action of one of a family of enzymes, nitric oxide synthases or NOS, converting the amino acid L-arginine to L-citrulline and forming nitric oxide in the process. Although many doubted that such a process could take place in living tissue, the horseshoe crab, for example, depends on the L-arginine:nitric oxide process to prevent its blood cells from aggregating.

This research overturned some basic views of the cardiovascular system whereby blood pressure was seen as resulting from a constant balancing between factors influencing the constriction and the dilation of blood vessels. Changes in blood pressure and blood flow happened if the balance was tipped too far one way or the other. Now, it seems, the normal cardiovascular state is tilted in one direction, and the dilation of vessels is sustained by a steady flow of nitric oxide. So any interruption to the production of nitric oxide interferes with the tone of the smooth muscle.

If the normal state of blood vessels is to be dilated constantly, then the prevailing perception of blood pressure and the approach to managing hypertension may need revision. Raised blood pressure may therefore be as much a problem of a lack of dilator tone as it may be due to constriction caused by some unknown factor.

This new insight also explains the observation made more than a century ago that a group of drugs, based on amyl nitrite and nitroglycerine, could stop a painful attack of angina—the chest pain now known to be caused when the heart muscle is short of oxygen. By chance, Victorian physicians had determined that although it was too dangerous to give people nitric oxide directly, substances that released it slowly could relieve hypertension. The helpful effect on blood pressure of a whiff of amyl nitrite vapour was recognized as long ago as 1867, and Conan Doyle credited Sherlock Holmes with that knowledge in *The Case of the Resident Patient*.

The poisonous effects of nitric oxide were well known. It was easy enough to make in the laboratory by adding copper turnings to concentrated nitric acid and collecting the colourless gas over water. It nearly killed Sir Humphry Davy in 1800.

In World War I, doctors noticed that workers packing shells with nitroglycerine in ammunition factories had very low blood pressures. The observation led to the development of a pill containing nitroglycerine, that remains effective as an emergency vasodilator when placed under the tongue to give rapid relief for angina. Although effective, the precise way in which the nitric oxide is released from nitroglycerine to imitate the L-arginine source of the molecule is still a mystery. Nitric oxide is changed rapidly once in the bloodstream because it is readily bound to the iron in haemoglobin.

As research into nitric oxide gathered momentum nine years ago, investigations spread way beyond the effect of the endothelially derived molecule. Three forms of the NOS enzyme were identified: one in the endothelium, one in the brain and one in the immune system. Moreover, biochemists were intrigued to discover that these enzymes were unusual in that they controlled a two-stage reaction that would usually take two enzymes.

Clinically, there are far-reaching implications for nitric oxide treatment of various forms of cardiovascular diseases. A vast range of research is currently directed towards transferring the laboratory and animal findings on nitric oxide for the benefit of cardiovascular and heart disease sufferers.

In cases involving a risk of heart attack, attention focuses on nitric oxide deficiency, and the dangers when its release is blocked from a diseased coronary artery so that the vasodilator tone needed to regulate the flow of blood is lost. A trace of nitric oxide gas (25 p.p.m.)

inhaled by patients with pulmonary hypertension can relieve lung congestion. In a treatment for newborn babies, breathing problems are being helped by the inhalation of nitric oxide, which relaxes constricted blood vessels and dilates the lung's blood vessels.

Generally, low blood pressure is not a problem in healthy people. Occasionally, it is a symptom of a serious condition, and an acute drop can signal that an overwhelming infection has caused septic shock and severe tissue damage. Septic shock depresses blood pressure. The loss of blood flow can cause tissue damage which in turn increases the production of nitric oxide, leading to a further fall in blood pressure. Low blood pressure induced by septic shock has been restored with a treatment that included the use of an NOS inhibitor.

The remarkable role nitric oxide plays as a messenger between nerve cells was revealed by John Garthwaite and colleagues at Liverpool University, who first identified it in the brain. Subsequent measurements have shown that the brain contained more of the nitric oxide synthase enzyme than any other organ.

When research into the possible role of nitric oxide in the central nervous system began, the brain was the organ least expected to contain the molecule. It transpired that the nitric oxide synthase enzyme was not confined to small areas, but was distributed throughout the brain, suggesting an involvement in almost every brain function. It turns out that because the molecule is so small, it is a physically convenient messenger that diffuses into and out of cells easily, and it is now a prime candidate for the much searched for 'retrograde messenger' that is the basis of memory.

Animal studies suggest that an effector cell in the brain which releases the chemical messenger glutamate can stimulate the receptor cell with this chemical to release nitric oxide. If it is strongly stimulated, the receptor sends back a nitric oxide molecule to tell the sender that the message has been received, and programmes it to send an even stronger signal next time—the phenomenon of long term potentiation that is thought to be linked to memory formation.

Nitric oxide produced in the brain by the neuronal form of the nitric oxide synthase acts as a chemical messenger at the synapses. *In vitro* and *in vivo* animal experiments showing the role of neuronal nitric oxide in memory have opened a new approach to studies of Alzheimer's and Parkinson's diseases, as well as other neurological disorders. Too much nitric oxide, on the other hand, may be responsible for killing brain cells in conditions such as stroke.

In yet another role, nitric oxide helps the immune system's macrophages—the cells in the body that are activated in injury and illness to remove invading microorganisms and other cells—when they seek out invading bacteria or cancer cells to destroy. The macrophages use the cytotoxic properties of nitric oxide to sweep up parasites, bacteria and other potentially infectious agents.

Prof. Eddy Liew's work on the role of nitric oxide in the immune system shows that the molecule will destroy many organisms that are difficult to kill by other means. His group has also demonstrated the susceptibility to nitric oxide of the vicious parasite that causes Leishmaniasis, a group of potentially fatal tropical diseases caused by parasites transmitted by sandfly bites.

Research on nitric oxide, its physiological and pathological roles and clinical potential is currently one of the most exciting areas of biochemistry and biology.

On 31 May 1995, the Royal Society of London and the Association of British Science Writers held a scientific press briefing on nitric oxide. The above article is a summary of some of the discussions.

Equivalence of the velocity of sound in water and ice at mesoscopic wavelengths

This is the title of a paper recently published in *Nature* (G. Ruocco, F. Sette, U. Bergmann, M. Krisch, C. Masciovecchio, V. Mazzacurati, G. Signorelli and R. Verbeni *Nature* 1996, **379**, 521–523) by a group of scientists working at the European Synchrotron Radiation Facility, Grenoble, France. These scientists have observed the inelastic scattering of intense monochromatic X-ray beams from H_2O in both its solid and liquid forms. The X-rays used are produced from the synchrotron and are chosen with a wavelength between 5 Å and 3 Å. These wavelengths correspond to the intermolecular distances observed in the samples of interest and allow the scientists to investigate the molecules' intermolecular dynamics. The X-ray beams are monochromatized in a *tour de force* and inelastic scattering, reminiscent of Raman scattering, observed from the condensed phases. The observed excitations, between +20 meV, $\approx$160 cm^{-1}, and –20 meV, correspond to collective oscillations of water molecules—akin to phonons observed in solid-state Raman spectra with both Stokes and anti-Stokes lines.

In general, the dynamics of density fluctuations within the condensed phase are measured by inelastic neutron scattering and are represented by the function $S(Q, \omega)$ which defines the scattering dependence of momentum transfer, Q, and energy transfer, ω, between the scatterer and incident neutron. Features in $S(Q, \omega)$ are related to excitations or oscillations with wavelength $2\pi/Q$ and frequency ω. When the condensed phase is probed with radiation of long wavelength (long with respect to the structure of the molecules present) then one probes the macroscopic structure of the medium and observed excitations corresponding to sound or acoustic waves which acts as a pressure wave compressing the molecules.

Measurements of $S(Q, \omega)$ in the energy–momentum region of interest here, 0.1–20 meV and 0.01–10 nm^{-1}, respectively, are normally made by neutrons. Neutrons are heavy and can consequently transfer large amounts of momentum, they may also be readily monochromatized, but with a loss of flux—the narrower the energy distribution of neutrons emitted by a source such as a nuclear reactor the fewer neutrons it con-

tains. However, individual neutrons may be counted, and if sufficient time is available for counting low scattering levels, reasonable statistics may be obtained. Inelastic scattering experiments may also be performed with X-rays. However, because of the much lower mass of the photon, to observe the same momentum transfer as with neutrons one must use very energetic photons—X-rays. The problem then becomes one of producing sufficiently well monochromatized X-rays. The present authors measured $S(Q, \omega)$ for water with X-rays at about 18 000 eV looking for narrow excitations in the region of 20 meV. That is, looking for an energy resolution in the scattered X-rays of 1 part in 10^7. This is possible if one is prepared to sacrifice flux—the narrower the energy distribution/wavelengths of X-rays emitted by a source such as a monochromator, the fewer photons it contains. In the present experiment, the authors used a curved mirror of 7 m radius to capture the inelastically scattered photons and to reflect them to a detector.

Spectra were determined at a number of different momentum transfers, and the dispersion in the frequencies of the excitations was determined. These measurements indicated that, in H_2O there exits a space–time domain (a region of energy and momentum transfer) where the interparticle correlations (intermolecular vibrations between individual H_2O molecules) are very similar in both ice and liquid water. That is, there was no discernible difference between the measured dispersion relationships for solid or liquid water. Indicating that in the range of momentum transfer investigated, that is, over a particular length-scale, collective longitudinal excitations propagate with the same velocity in liquid water as in ice (253 K). This of course raises the interesting question as to what is the difference between a solid and a liquid composed of the same molecules.

It is generally assumed that sound travels faster in the solid phase of a material that in its liquid phase. This is certainly true for waves of macroscopic wavelength, the dynamics of which depend upon the elastic properties of the medium and hence on any long-range order that may be present. At wavelengths approaching typical interparticle distances, in contrast, the dynamics should become insensitive to the long-range organization of the medium.

We could say that the liquid and solid states are thermodynamic concepts related to the time evolution of the relative positions of the constituent molecules. Whereas in the solid there are no changes over a long time-scale, the liquid is characterized by the diffusive motion of constituent molecules on short time-scales. This is what is observed—in the solid the molecules are locked in place. In a liquid, the molecules are free to diffuse—the energy 'locking' a molecule in a particular configuration is of the same order as the available thermal energy, kT, and so when one molecule collides with another molecule all local configurations are lost. This is, however, a picture of the condensed phase at large distances. At microscopic distances within the material, for processes such as local bonding, proton exchange and nearest neighbour distances, the difference between the liquid and the solid phase often becomes irrelevant to the particular physical problem. In the intermediate or mesoscopic domain, characteristics such as bond formation, chemical reactions and aggregation of complex systems, density fluctuations in the liquid and solid phases, may deviate from macroscopic behaviour, although they still involve many atoms.

These results indicate that despite the fundamental structural and dynamical differences between liquid water and ice, the dynamical response of the two phases is strikingly similar at short probing wavelengths. Perhaps on these very small length scales, liquid water behaves as a semi-crystalline material—the waves probing, in both cases, the network of hydrogen bonds which characterize condensed H_2O.

Eighth International Conference on Phenothiazines and Structurally Related Phychotropic Compounds

This meeting was organized over 26–29 February 1996, by the Chemistry Department of Rajasthan University, Jaipur, India, and held in the Clarks Amer Hotel, Jaipur. The Confernce was under the chairmanship of Dr R. R. Gupta. There were 9 plenary and 19 invited lectures in addition to the 12 oral and 50 poster presentations. The lectures and posters covered the follwoing topics:

- Physical and chemical aspects;
- Analytical aspects and advances in assay methodology;
- Advances in drug metabolism;
- Toxicological aspects;
- Progress on mode and site of action;
- Clinical pharmacology and structure/activity relationships;
- Drug interactions with other drugs or macromolecules and therapeutic complications; and
- Present and future in microbiology and cancer.

This multidisciplinary conference, involving chemistry, biology, life sciences, clinical and pharmaceutical chemistry, was the first of its series to be held in a developing country. The meeting was attended by 150 delegates, from numerous countries, who were unanimous in their praise of the scientific and social content.

Delagates to the 8th International Conference on Phenothiazines and Structurally Related Compounds.

Dismantling chemical weapons. Joseph Bunnett '42 collaborates with international scientists in weapons destruction

The following is an abbreviated version of an article which appeared in the alumni magazine of Reed College, Oregon, USA, about one of its respected members—Prof. J. Bunnett (class of 1942). The author is Laura Alvarez.

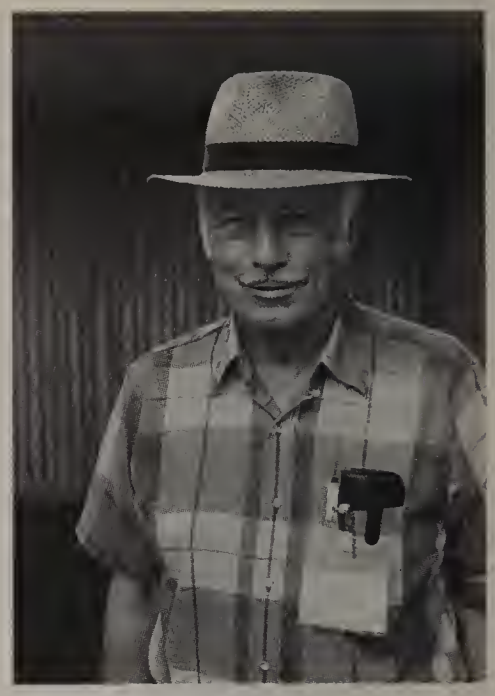
A Russian farmer encounters an unidentifiable, corroded metal can in his field one day. Upon opening it, he is overwhelmed by the toxic mustard gas that has developed over the past 75 years; breathing in the gas, the farmer's lungs are severely blistered.

Such unexploded chemical munitions continue to be found in European countries on former World War I battlefields. In addition, many governments around the world still have stockpiles of such munitions and don't know how best to destroy them. The United States government has declared that it possesses 30 000 tons of chemical weapons—a number surpassed only by the Russian government's holdings. The Japanese government has recently acknowledged its obligation to clean up the stockpiles of chemical weapons it abandoned in China in 1945. Reed trustee Joseph Bunnett is working with international coalitions of scientists in developing the technologies needed for destroying such weapons.

Currently an emeritus professor of chemistry at the University of California at Santa Cruz, Bunnett's involvement in chemical weapons destruction encompasses three separate projects. For the past 4 years, he has served as chairman of the committee on chemical weapons destruction technologies of the International Union of Pure and Applied Chemistry (IUPAC). This union is the 'international high organization of chemistry'; members are not people but national chemical societies—US membership is through the National Academy of Sciences.

In part, Bunnett's committee has been giving attention to issues that were until recently unrecognized by military authorities or thought to be politically unwise to study. To some extent, the committee's recommendations have been met with a diffident response. A positive development in this matter, however, has been the recruitment of Graham S. Pearson, recently retired Director General of the UK Chemical and Biological Defence Establishment, and his willingness to chair an evaluation of technologies for the destruction of chemical weapons. Because of Pearson's eminence and the growing world-wide interest in the outcome of that evaluation, the committee's work is now expected to be easier. Many nations that possess chemical weapons will be required by the Chemical Weapons Convention's multinational treaty to destroy them within 10 years.

Bunnett's second project is his collaboration with Polish scientist Marian Mikolajczyk, also a member of the IUPAC committee. The two scientists were awarded a USD 48 000 grant from NATO to conduct an advanced research workshop in Lodz, Poland, this spring, studying the chemical problems associated with old arsenic and mustard munitions. Arsenic weapons are especially dangerous because the arsenic component cannot be destroyed. Mustard gas, which is in the form of an oil, can be converted to other fairly innocuous chemicals. However, after sitting in a battlefield or on a shelf for 50–80 years, the mustard liquid gels partly and generates a gas; sometimes when the container is opened, this gas can cause a fountain effect, spraying out the toxic mustard gas.



Joseph Bunnett

The third component of Bunnett's recent work in this area is serving as the chairman of the Peer Review Committee for the Russian American Joint Evaluation Programme. The US government organized this programme to evaluate the Russian technologies of destroying chemical weapons before deciding which technology to support in helping the Russians in their weapons destruction. Both countries' militaries are sponsoring the collaboration of Russian and American scientists conducting experiments to test the Russian technologies. The peer review committee consists of both Russian and American scientists who are not affiliated with the military, critiquing the evaluation experiments for their scientific quality. Bunnett especially appreciates the personal interaction with Russian scientists over shared personal values and professional interests: 'of course there are some differences, in the liquor we drink, and maybe some differences in style of clothing, but not really big differences. So far as the more important things are concerned, personal values and things of that sort, I don't see a difference.'

Bunnett has appreciated this component of international collaboration and travel in various visiting professorships at such places as the University of Buenos Aires, Argentina; the University of Canterbury, in Christchurch, New Zealand; and Tohoku, Tokyo, and Osaka Universities in Japan. He has also traveled under fellowships, including a Fulbright at University College in London and a Fulbright and Guggenheim at the University of Munich in Germany.

Although Bunnett's recent work is different from the research he undertook as a professor, he did gain some preparation for it in some of his earlier work. He served on a National Research Council committee surveying alternatives to incineration as a means of destroying chemical weapons. He also served on a governmental panel that determined that the 'Gulf War Syndrome' was not caused by exposure to chemical weapons.

Update on the IUPAC Division of Chemistry and the Environment

Further to the announcement by the then Secretary General of IUPAC, Prof. Gerrit den Boef, of the creation of two new Divisions of **Chemistry and the Environment** (DCE) and **Chemistry and Human Health** (*Chemistry International* 1995, 17, 230–232) we can now provide an update on the structure and activities within the DCE.

The new Division comprises a combination of the previous Applied Chemistry Division (VI) and Commission V.9, namely Environmental Analytical Chemistry from the Analytical Chemistry Division. There has also been some refocusing of the activities of some Commissions within the Division to further emphasize the environmental aspects of their work. The DCE comprises six Commissions which are described below:

- Commission VI.1 (former V.9)—Fundamental Environmental Chemistry
- Commission VI.2 (former VI.4)—Atmospheric Chemistry
- Commission VI.3 (former VI.6)—Soil and Water Chemistry
- Commission VI.4 (former VI.5)—Agrochemicals and the Environment
- Commission VI.5 (former VI.1)—Food Chemistry
- Commission VI.6 (former VI.3)—Oils, Fats and Derivatives

The President of the DCE is Dr Junshi Miyamoto (Japan), the Vice-President is Prof. Werner Klein (Germany) and the Secretary is Dr Terry Roberts (UK).

This new Division is best placed to provide unbiased, authoritative reviews on the behaviour of chemical compounds in the environment and make a valuable contribution to global sustainable development. Some time was spent at the General Assembly in Guildford (1995) discussing the terms of reference of the DCE which is committed to promotion of intra- and inter-divisional collaboration on all matters pertaining to the environment. The DCE is charged with further improving coordination of all environmental activities within IUPAC.

The major change is the incorporation of Commission V.9 into the 'Applied Chemistry' activities. The DCE will therefore undertake both fundamental and applied chemistry projects aimed at solving environmental problems. Moreover, it is recognized that the concepts and analytical techniques related to fundamental aspects of environmental chemistry (to be studied by Commission VI.I) are pervasive and will be relevant to all the other, Applied Chemistry Commissions. The rationale for this structure is that the fundamental concepts are independent of the nature of the environmental compartments and can therefore be studied in isolation in Commission VI.1 whereas their interaction with various macroscopic processes can be studied in the specific Commissions.

There is, of course, inevitable overlap between Commissions VI.2 to VI.6 and this will encourage development of multidisciplined projects. For example, common issues have been identified within the Soil and Water Chemistry Commission and the Agrochemicals and the Environment Commission and it is important for these two expert groups to combine their experience to produce the broadest possible perspective as the IUPAC view. A specific example is the major issue of pesticides in natural waters in which the Agrochemicals Commission would focus on understanding and assessing means of predicting movement of pesticides to water while the Soil and Water Commission would deal with the issue of removal of pesticides from water. Both Commissions have also been involved with analytical methodologies for trace levels of pesticides in the environment and this is clearly an area in which the Fundamental Environmental Chemistry will continue to play a vital role.

The DCE will also focus its terms of reference on other important areas, for example, improving our understanding of intra- and inter-compartmental fluxes of chemical compounds in the environment. Links between micro- and macro-scale processes will also be studied. With reference to the Commissions on Food Chemistry and Oils, Fats and Derivatives, investigations will be made of the pathways of chemicals in the environment to include the influence of the environment on food quality. In addition, the integration of fundamental environmental chemistry into the DCE will allow the more efficient development and critical evaluation of physical chemical parameters and concepts, analytical methodologies and interpretation of data.

Interaction between IUPAC and other international organizations is, of course, actively encouraged, not only to ensure the necessary collaboration and support from IUPAC but also for IUPAC to prioritize its efforts to deal with issues that it is uniquely placed to manage. To this end, there is ongoing collaboration with SCOPE, WHO and FAO. Dr Miyamoto represents IUPAC at a number of international meetings including the IFCS (Intergovernmental Forum on Chemical Safety) meeting on Persistent Organic Pollutants in Canberra in March (1996), and IPCS (International Program on Chemical Safety) meeting on the future direction of world-wide chemical control in Washington, DC, in October.

The DCE Commissions continue to be encouraged to undertake outreach programs of which there have been several excellent programs in recent years. For 1996, there are two major meetings planned and encouraged by IUPAC. The Commission on Atmospheric Chemistry is holding a workshop on 'Workstation Measurement Techniques in Atmospheric Chemistry' to be held in Salvador/Bahia, Brazil during November 1996 and a workshop on 'Pesticide Uses and Environmental Safety in Latin America' is to be held by the Agrochemicals in the Environment Commission to take place in Sao Paulo, Brazil during 14–16 October 1996.

There is therefore every opportunity and encouragement from IUPAC in general and from the DCE Committee for the internationally recognized scientists from industry, academia and national or government institutes within the DCE Commissions to collaborate in the unique way that IUPAC combines such a cross-section of views.

A more detailed article about the work of the DCE is in preparation.

T.R. Roberts & J. Miyamoto

Names and Addresses

Full details (names, addresses, telephone/telex/Fax numbers and E-mail) of the officers of IUPAC bodies were published in *Chemistry International* 1995, **17**(6), 215–226. The IUPAC Secretariat have been notified of the following changes:

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Prof. Irina Beletskaya (Chairman, Monographs for the 21st Century) E-mail: beletska@elorg.chem.msu.su

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Prof. Sandra Rondinini Cavallari (Secretary, Commission V.5) Tel.: +39 226 603 217; Fax: +39 226 603 217: E-mail: vertova@icil64.cilea.it

Prof. Thomas T. Tidwell (Chairman, Commission III.2) Department of Chemistry, University of Toronto, Toronto, Ontario M5S 3H6, Canada.

Commission on Biotechnology (attached to bureau during 1996–1997)

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New Publications

Health and safety guides

The Environmental Health Criteria (EHC) monographs produced by the International Program on Chemical Safety (IPCS) include an assessment of the effects on the environment and on human health of exposure to a chemical or combination of chemicals, or physical or biological agents. They also provide guidelines for setting exposure limits.

The purpose of a Health and Safety Guide (HSG) is to facilitate the application of these guidelines in national chemical safety programmes. The first three sections in a HSG highlight the relevant technical information in the corresponding EHC. Section 4 deals with advice on preventive and protective measures and emergency action; health workers should be thoroughly familiar with the type of information found in this section. The section on regulatory information has been extracted from the legal file of the International Register of Potentially Toxic Chemicals (IRPTC) and from other United Nations sources.

Two new guides have recently been published, they are:

Health and Safety Guide no. 100, Cresols (ISBN 92 41511 00 1)

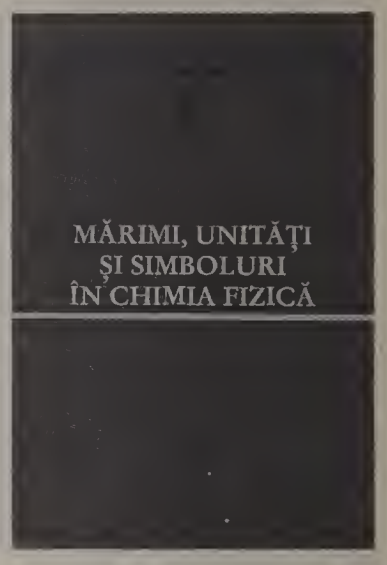
Health and Safety Guide no. 101, Hydroquinone (ISBN 92 41511 00 1 X)

Published by the World Health Organization for the International Program on Chemical Safety.

These publications are priced CHF 5 in developed countries and CHF 3.5 in developing countries. Further information and copies are available from: Distribution and Sales, World Health Organization, 1211 Geneva 27, Switzerland.

Translation of the 'Green Book' into Romanian

Quantities, Units and Symbols in Physical Chemistry has been translated into Romanian under the auspices of the Academia Romana, copies are available from; Dr D. I. Marchidan, Institute of Physical Chemistry, Splaiul Independentei 202, Bucharest 77208, Romania.



Macromolecular symposia

The IUPAC International Symposium on Polymer Morphology and Electrical Properties was held on 5–7 July 1995 in Łodz, Poland. These symposium have been organized in order to bring together scientists and engineers active in the field of polymer structure and morphology with those engaged in studying electrical properties of dielectric, semiconducting and conducting polymers.

The occasion for this 3-day symposium was also the 70th birthday of Prof. Marian Kryszewski, Centre of Molecular and Macromolecular Studies, Polish Academy of Sciences in Łodz, Poland. His scientific interest concentrated for many years on the fields closely covered by the Symposium programme.

From all over the world, 110 researchers from both

IUPACSEARCH Version 4.2

A free computer disk containing abstracts of all IUPAC recommended nomenclature and symbols and technical reports published in *Pure and Applied Chemistry* from 1960 through to the end of 1995 is now available. The disks are 3½", high-density, IBM-PC compatible format, will run under DOS (version 3.3 or later) and under Windows (although it is not a Windows version and does not use the mouse). A hard disk with 7 Mb of free space is required. The software allows for Boolean searches; it is menu-driven and easy to use. Both colour and mono-monitors are supported. Sorry, a Macintosh version is not available.

Please e-mail or Fax your request to: Mrs Gwyneth Pettit, Fax: +44 194 388 0310; E-mail: acadsoft@bcs.org.uk

academic and industrial institutions took part in the Symposium. 18 plenary lectures, 24 contributed papers and 58 posters were presented. The success of this symposium was insured by the presence of many distinguished scientists and by high quality of presentation.

Most of the presented papers are published in a special volume of *Macromolecular Symposia (Macromolecule–Metal Complexes)*, Vol. 104, March 1996; Hüthig & Wepf Verlag; ISSN 1022-1360.

The IUPAC 6th International Symposium on Macromolecule, Metal Complexes (MMC-VI), was held in Guangzhou China on 2–5 November 1995. The symposium was attended by 102 active chemists from 12 countries all over the world discussing the frontier topics relevant to macromolecule—metal complexes:

1. Synthesis, characterization and properties; 2. Electron and ion conducting and electrochemical behaviour; 3. Gas, liquid and metal absorption, transportation, separation, and sensors; 4. Photosensitive and temperature-sensitive materials; 5. Catalysts and reagents; 6. Liquid crystals; 7. Biochemical behaviour and medical application.

The 36 presented papers are published in a special volume of *Macromolecular Symposia (Macromolecule–Metal Complexes)*, Vol. 105, March 1996; Hüthig & Wepf Verlag; ISSN 1022-1360.

The International Symposium on Ionic Polymerization sponsored by IUPAC and Istanbul Technical University was held on 4–8 September 1995, in Istanbul.

The symposium was attended by 150 scientists from 23 countries. For the first time, the former series of meetings on cationic, anionic and ring-opening polymerizations were grouped together as Ionic Polymerization. A prestigious group of speakers from each field was gathered together for this combined symposium. Many of the speakers commented how much more appropriate was a combined symposium, than several smaller individual meetings.

The scientific programme included recent developments on the following aspects of ionic polymerization:

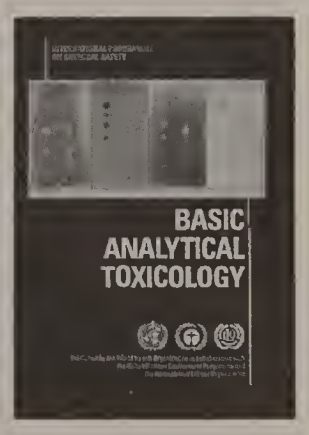
1. Fundamental chemistry and mechanism; 2. Controlled polymer synthesis; 3. Telechelics, Macromonomers and Block and Graft Polymers; 4. Kinetics and modelling; 5. Industrial applications; 6. Light-induced processes.

The 29 presented papers are published in a special volume of *Macromolecular Symposia (Macromolecule-Metal Complexes)*, Vol. 107, April 1996; Hüthig & Wepf Verlag; ISSN 1022-1360.

The 36th Microsymposium on Macromolecules: High-Swelling Gells, was held in Prague on 10–11 July 1995.

The 16 presented papers are published in a special volume of Macromolecular Symposia *(Macromolecule-Metal Complexes)*, Vol. 109, May 1996; Hüthig & Wepf Verlag; ISSN 1022-1360.

Basic analytical toxicology



This book provides a practical guide to the laboratory analysis of over 100 substances frequently involved in episodes of acute poisoning. Noting that many hospitals, especially in developing countries, lack the support of analytical toxicology services, the book aims to help laboratory staff perform a range of simple tests known to produce rapid and reliable results for the management of poisoning emergencies. All tests described can be performed without the need for sophisticated equipment, expensive reagents, or a continuous supply of electricity.

The manual opens with general information about the organization and functions of an analytical toxicology laboratory, the principles of safe laboratory practice, and the essentials of emergency medicine and intensive care that will influence the laboratory's work. A brief introduction to the apparatus, reference compounds and reagents needed in the laboratory is followed by an explanation of basic clinical issues. Details range from a table listing the clinical features associated with some common poisons to a description of essential symptomatic and supportive measures that can be taken before the diagnosis is confirmed.

Chapter three explains the most useful biochemical and haematological tests for the diagnosis of acute poisoning and for assessment of prognosis. The final introductory chapter goes through the do's and don'ts of laboratory practice pertaining to safety, the performance

of colour tests, the pre-treatment of samples, and procedures for the use of thin-layer chromatography and ultraviolet and visible spectrophotometry.

The remaining two chapters, which constitute the core of the manual, describe the many simple analytical tests that can be used to detect and identify poisons, whether in biological fluids or in powders, tablets, or other items found near the patient. The first chapter, on qualitative tests for poisons, sets out a three-part series of tests designed for use as a routine, rapid screen, especially appropriate in the many cases where the identity of the poison is unknown.

The second and most extensive chapter provides step-by-step instructions for the performance of qualitative tests and some quantitative methods for 113 specific poisons or groups of poisons. Substances covered range from pesticides and other industrial chemicals, through compounds contained in household products, to pharmaceuticals, plant toxins and commonly abused drugs. To assist communication between the toxicologist and the clinician, each monograph also contains information on clinical signs of intoxication and recommended treatment. All techniques and procedures have been tested by laboratory technicians in developing countries to assure reliable performance using relatively simple apparatus.

Basic Analytical Toxicology *(R. J. Flanagan, R.A. Braithwaite, S. S. Brown, B. Widdop & F.A. de Wolff). Published by the World Health Organization, 1995, xii + 274 pages + 8 colour plates (available in English; French in preparation) ISBN 92 415 4458 9; CHF 60./ USD 54.00, In developing countries: CHF 42.*

Committee on Data for Science and Technology (CODATA)

CODATA is an interdisciplinary scientific committee of the International Council of Scientific Unions (ICSU) which seeks to improve the quality, reliability, management and accessibility of data which is considered of importance to all fields of science and technology. The general objectives are:

- Improvement of the quality and accessibility of data, as well as the methods by which data are acquired, managed and analysed.
- Facilitation of international cooperation amongst those collecting, organizaing and using data.
- Promotion of an increased awareness in the scientific and technical community of the importance of these activities.

The major classes of activities undertaken by CODATA in addressing the above objectives are:

- Preparation of key data sets for which consistent international use is desirable.
- Coordination of multinational projects.
- Creation of format standards to promote compatibility of datasets.
- Guidelines for the presentation of data in the primary literature.
- Supplying information on sources of reliable data.
- Education and training.
- Organization of conferences and workshops.

CODATA have just published their *Handbook* for 1996. This document contains information on Members, Task Groups, Commissions, Working Groups, and the Constitution and Publications of CODATA.

Further information may be obtained from the CODATA Secretariat, 51 Boulevard Montmorency, 75016 Paris, France; E-mail: codata@paris7.jussieu.fr and pg004@dial.oleane.com; World-Wide Web: http://www.cisti.nrc.c./codata/welcome.html

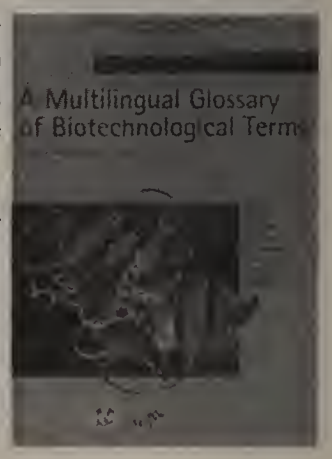
SCOPE Programme and Directory 1996–1998

SCOPE (Scientific Committee on Problems of the Environment) have produced a brochure describing their history, structure, program and goals. *SCOPE Programme and Directory 1996–1998* also consists of a series of varied individual projects, each addressing a significant scientific issue with specific goals. The three-cluster structure and the 17 ongoing projects are described in detail. Interaction of the projects is enhanced by a collective focus on sustainability.

The Membership of SCOPE, its 38 national members, 22 scientific associates and its constitution, are also included in this new brochure. A directory provides addresses and contact information for key individuals, the officers and members of the Executive Committee, national committee and scientific associate chairpersons and representatives, and chairpersons of the various projects.

Copies of this brochure may be obtained from the SCOPE Secretariat, Véronique Plocq-Fichelet (Executive Secretary), 51 boulevard de Montmorency, 75016 Paris, France; Tel.: +33 1 45 25 04 98; Fax: +33 1 42 88 14 66; E-mail: scope@paris7.jussieu.jr

Multilingual Glossary of Biotechnological Terms



This volume contains IUPAC-approved definitions of over 230 terms most frequently used in the multidisciplinary field of biotechnology (first published in *Pure Appl. Chem* 1992, **64**, 143–168), together with a translation of these terms into six languages, namely French, German, Japanese, Portuguese, Russian and Spanish. The terms

are presented in dictionary format for ease of reference.

This set of translations has been produced to facilitate communication between chemists, chemical engineers, biologists and bioengineers, and to render biotechnology more accessible to the chemistry profession in general. The scope of the contents includes the fields of microbiology, genetic engineering, biochemistry, molecular biology, biochemical engineering, bioprocessing and general concepts of biotechnology, thereby making this volume an indispensable source of reference.

Multilingual Glossary of Biotechnological Terms (H.G.W. Leuenberger, B. Nagel & H. Kölbl, eds). 1995, VCH, Postfach 10 11 61, D-69451 Weinheim, Germany; ISBN 3906390 13 6; 251 pages; DEM 78.

International Newsletter on Chemical Education, No.44

This issue of the International Newsletter contained a description of the 13th International Conference on Chemical Education (ICCE) held at the Inter American University of Puerto Rico in San Juan, 8–12 August, 1994. The programme listed 14 plenary lectures (two by Nobel Laureates), 118 symposium papers, 25 workshops and 7 'birds-of-a-feather' sessions. The academic programme was matched by an equally diverse and interesting social programme, and the only thing to mar such an excellent occasion was the island's drought. This may have inhibited the flow of water in the city's hotels, but not of ideas amongst the delegates.

The proceedings are now in print, but the following will give you just a hint of what the 13th ICCE had to offer. First, Angela Danil de Namor tells us about teaching and research activities in Latin America, and then Leonard Fine takes us into the fascinating world of the history of chemistry.

After 10 years in the Editor's chair, this is the last issue of the Newsletter to be edited by Peter Towse (CSSME, University of Leeds, Leeds, UK).

Teaching and research activities in Latin America

A.F. Danil De Namor (Department of Chemistry, University of Surrey, Guildford, Surrey GU2 5MI, UK)

Over the years, a considerable amount of effort has been extended by international organizations to bridge the gap between developing and highly industrialized countries. There is no doubt that a great deal of investment has been devoted to the training of graduates from the developing world at Master's and PhD levels. It is often found that this training has not been geared to the best benefit of the individuals or the countries involved, either because the research undertaken was not relevant to the needs of the country, or the Latin American institution does not have the funds required to acquire the research facilities needed by those who return to develop the research in which the training was given. The University of Surrey has taken a rather unconventional approach in initiating collaboration with institutions which do not have a research tradition. On this basis, long term projects in chemistry with well-established objectives have been developed, taking into account the fact that applied science requires basic science and if genuine help is to be given to developing countries this should be directed to providing the basis for ongoing research plans.

Thus, three MSc programmes have been established in Peru since 1984 in the following areas:

Chemistry at the National University of San Augustin

The aims are:

1 to provide up-to-date knowledge in the three branches of Chemistry (organic, inorganic and physical chemistry);
2 to emphasise the role of industry in the national economy by the introduction of two postgraduate courses in industrial chemistry; and
3 to provide the basis for future research initiatives by carrying out a research project as part of the requirements for this postgraduate degree.

Environmental Chemistry at the Catholic University of Santa Maria

Environmental science is a subject of world-wide concern for which chemistry forms a major component. In addition, the south of Peru is an important industrial region of the country and, as such, its population is exposed to serious contamination problems. Based on the international, national and regional importance of environmental issues, the first MSc programme in Environmental Chemistry in Peru was established in 1992.

The extraction of strategic metals at the National University of the Altiplano

Peru is a country with enormous mining resources for which the south contributes significantly with copper, tin, gold, molybdenum and other important metals. However, these resources have not been fully utilized due to the lack of both local expertise in this area and financial limitations. The support recently received from the European Union for a research project on gold extraction with the University of Surrey as a coordinator is directed to the training of young people in Europe and to the implementation of a research laboratory at the University of the Altiplano. This research initiative has motivated the establishment of the MSc programme on 'The extraction of strategic metals' in Peru. The aim of this postgraduate course is to produce highly qualified personnel able to cope with regional needs.

Problems associated with laboratory infrastructure and the lack of technical assistance still exist in Latin America. To overcome these problems, joint efforts from the international community are required and these should be addressed.

Lessons from history...and chemistry lessons

L.W. Fine (Department of Chemistry, Columbia University, New York, NY 10027, USA)

Introduction

In the nation created by legendary intellects such as Franklin and Jefferson, one might have expected governmental guarantees to go beyond life, liberty and the pursuit of happiness, and to include,...an appropriate education...embedded in a coherent curriculum, married to mathematics and science as much as to politics, art, music and literature. But there is no such governmental guarantee. Not in the Declaration of Independence. Not in the Constitution. Not in the Bill of Rights.

But guaranteed or not, as the USA enters its 3rd century, literacy is neither fully achieved nor sufficient. Chemistry teachers have always experimented with novel ways of increasing scientific literacy and improving the quality of life beyond the classroom. The 20-year experiment in computer-assisted instruction is about to bear fruit (arguably for the first time) that everyone can enjoy. Suddenly, powerful and wide-ranging graphics-based software programs, work-stations, smart terminals, Internet communications, and a host of multimedia and hypertext materials have infused new life into that experiment, propelling our chemistry lessons into a brave new world, making them more understandable as they become more visual. History-assisted instruction offers equally exciting opportunities for improving understanding of science and changing attitudes towards science.

Four chemistry lessons from history were presented:

1. Salvarson 606, Paul Ehrlich's magical bullet.
2. Trying to understand the existence of triphenylmethyl and the non-existence of hexaphenylethane.
3. Still stable after all those years: α, γ-bisphenylene-β-phenylallyl radical.
4. A polymer called polycarbonate.

All four are drawn from easily accessible sources in the scientific literature; all are designed to present the teacher with opportunities to teach concepts in contexts that go beyond the chemistry classroom; all offer students opportunities to explore the literature on their own and be more a part of the scientific processes earlier than might otherwise be thought possible; all are taken from the field of organic chemistry; all have been successfully used at Columbia in lower division undergraduate courses for first and second year students; and we believe our graduate student instructors and colleagues on the faculty have benefited from the experience these lessons have provided. Of these, and this is dictated solely by the limitations of space, two are described here.

Salvarson 606, Paul Ehrlich's Magical Bullet

In 1899, Paul Ehrlich was appointed Director of the Institute for Experimental Therapy in Frankfurt (Germany). The mandate Ehrlich set for himself was nothing less than establishing the fields of immunochemistry and chemotherapy, the former a matter of strengthening the body's defences and the latter a direct chemical attack on parasites afflicting a mammalian host. At the same time, giants of the German synthetic chemicals industry were busy manufacturing the items of their commerce: analgesics, antipyretics, anaesthetics...and pigments and dyes. This burgeoning activity characterized the growth of chemistry in that period.

For much of the 20 years before 1899, Ehrlich had been interested in the selective affinities of mammalian tissue. He discovered that certain dyestuffs stain disease-causing micro-organisms but not the tissue, and he was able to apply this principle to selective staining to living organisms. That, in turn, led to his histological staining methods and techniques for differentially staining white blood cells, methods and techniques still in use today, almost a century later.

Ehrlich first applied his selective staining principle to the problem of malaria. He was convinced that the same small molecules that stain cells preferentially on being admitted to the bloodstream would selectively join with pathogenic bacteria, killing them without harming the diseased body. In 1885, he reported that ethylene blue (methyl thinning chloride) was effective in just that way.

Turning to organic compounds of arsenic, Ehrlich was the first to describe the correct chemical structure of Atoxyl (sodium sanilate) which had shown considerable promise in the treatment of sleeping sickness and syphilis, though not without dangerous side-effects. As he described it, his therapeutic programme 'consists of all kinds and varieties, from substances having a certain effectiveness to investigate the action of each and, building on the results thus obtained, to arrive at ever better therapeutic agents. This means learning to aim, and doing so by means of chemical variation.' Working with a Japanese physician, Sahachiro Hata, Ehrlich was able to predict and demonstrate the effects of Salvarson 606 (3,3′-diamino-4,4′-dihydroxyarsenobenzene). Salvarson was the first sure-fire treatment for syphilis and other infectious diseases caused by spirochetes, as well as trypanosomes (protozoa). It was the first triumph of chemotherapy.

Still stable after all those years: the α, γ bisphenylene-β-phenylallyl radical

In experimental work while a National Research Council Fellow at Harvard during 1931–32, C. Frederick Koelsch prepared and described the properties of the α, γ bisphenylene-β-phenylallyl radical. A paper setting down the details of the work was submitted to the editors of the Journal of the American Chemical Society but it was not accepted for publication. The referees' report held that the properties of the principal compound could not be those of a radical.

In what can only be described as a once-in-a-lifetime opportunity, Koelsch was able to publish his original paper 27 years later. It stands as a deliciously understated counterpoint in history, unchanged from the original except for three footnotes. He closed with the wry observations that a sample kept in air for 27 years is unchanged in appearance, that it shows a high free radi-

cal content, that the structure originally suggested appears to be unequivocally confirmed, and that in the interests of historical accuracy, the original paper is published unchanged!

The message is to use lessons from history in teaching chemistry. It leads to a better understanding of the processes of chemistry, the nature of the physical sciences, and contexts in which useful (and useless) results are obtained. Knowing something about how events unfolded may help nonscientists deal with science in life and present the lives of scientists in a more realistic and lively manner. Use history lessons often. Use them thoughtfully. But use them.

Recent Reports

In this section we publish summaries of the most recent IUPAC recommendations on nomenclature and symbols and technical reports. The full texts of these recommendations and reports are published in *Pure and Applied Chemistry*.

Acronyms used in theoretical chemistry

Synopsis

An alphabetic list of acronyms used in theoretical chemistry is presented. Some explanatory references have been added to make the acronyms more understandable, however, still more are required. Critical comments, additional references, etc. are requested.

This document was prepared for publication by R.D. Brown, J.E. Boggs, R. Hilderbrandt, K. Lim, I.M. Mills, E. Nikitin and M.H. Palmer from the Working party on Theoretical and Computational Chemistry of the Physical Chemistry Division. Comments should be sent to the coordinator of this project: Prof. Ronald D. Brown, Chemistry Department, Monash University, Clayton, Victoria 3168, Australia, Fax: +61 3 9905 4597 and E-mail: rdbrown@vaxc.cc.monash.edu.au. The full details are to be found in Pure Appl. Chem. *1996, **68**, 387–456.*

Symmetry, selection rules and nomenclature in surface spectroscopies (IUPAC Recommendations 1996)

Synopsis

The widespread use of techniques such as vibrational spectroscopy and photoelectron spectroscopy for the investigation of adsorbates on single crystal surfaces has focused attention on the symmetry properties of adsorbed molecules and on the application of selection rules. In much published work, however, confusion exists as to the appropriate point groups and, in the case of ordered overlayers, the appropriate space groups. In this document, the symmetry properties of clean and adsorbate-covered single crystals are described, appropriate nomenclature suggested and the physical principles leading to selection rules in surface spectroscopies briefly listed.

This Report was prepared for publication by A.M. Bradshaw[1] and N.V. Richardson[2] ([1]Fritz-Haber-Institute der Max-Planck-Gesellschaft, Faradayweg 4–6, 14195 Berlin, Germany and [2]IRC in Surface Science, University of Liverpool, PO Box 47, Liverpool L69 3BX, UK) for the Commission on Molecular Structure and Spectroscopy of the Physical Chemistry Division. The full details are to be found in Pure Appl. Chem. *1996, **68**, 457–467.*

Stability constants of metal complexes of amino acids* with charged side chains. Part I: Positively charged side chains† (Technical Report)

Synopsis

The stability constants of the proton and metal complexes of the basic α-amino acids arginine, lysine, and ornithine have been collected and critically evaluated on the basis of the considerations of the factors affecting the stability constant's determination, such as experimental method, conditions of measurement, purity of reactants, calibration of apparatus and method of calculation. In the presence of the side chain basic group, metal complex formation normally occurs through the glycine-like mode of coordination by the amino acids with the side chain group protonated, and deprotonation from the complexes often occurs in basic solution. The collected stability constants were evaluated as 'recommended', 'tentative', 'informative', 'doubtful' or 'rejected' according to the above criteria. The thermodynamic parameters reported for a limited number of complexes have also been collected and evaluated.

*Although IUPAC nomenclature recommends 'aminocarboxylic acid', the expression 'amino acid', more familiar to biochemists to whom this review is primarily addressed, has been used throughout.

† Series Title: Critical Evaluation of Stability Constants of Metal Complexes in Solution

This Report was prepared for publication by O. Yamauchi and A. Odani (Department of Chemistry, Faculty of Science, Nagoya University, Nagoya, 464–01 Japan) for the Commission on Equilibrium Data of the Analytical Chemistry Division. The full details are to be found in Pure Appl. Chem. *1996, **68**, 469–496.*

Glossary of terms in quantities and units in clinical chemistry (IUPAC–IFCC Recommendations 1996)

Synopsis

From 1967 onwards, a number of documents have been published prepared by IUPAC/C–QUCC and IFCC/C–QU (from the beginning of 1996 C-NPU), with input from many clinical chemistry laboratory scientists world-wide, and consistent with standards promulgated by authoritative international scientific organizations. Because of the importance of a consistent terminology in clinical chemistry and because these documents are often published in journals that may not be readily accessible, the C-NPU has prepared a glossary containing those terms considered of particular interest to the clinical chemistry and clinical laboratory science communities. The glossary has been compiled from definitions taken from published documents of the C-NPU. It also contains a number of terms and their definitions, considered relevant to the practise of clinical chemistry, taken from the official documents of other commissions of IUPAC and of international science organizations such as the International Organization for Standardization, the International Bureau of Weights and Measures and the International Union of Biochemistry and Molecular Biology.

*This Report was prepared for publication by H.P. Lehmann[1], X. Fuentes-Arderiu[2] and L.F. Bertello[3] ([1] Louisiana State University Medical Centre, New Orleans, Louisiana, USA, [2] Ciutat Sanitària i Universitària de Bellvitge, L'Hopitalet de Ilobregat, Barcelona, Spain, [3] Perú 420, 1640 Martínez, Buenos Aires, Argentina) for the Committee on Quantities and Units of the International Federation of Clinical Chemistry and for the Commission on Quantities and Units in Clinical Chemistry of the Division of Chemistry and Human Health. The full details are to be found in Pure Appl. Chem. 1996, **68**, 957–1000.*

Glossary of terms relating to pesticides (IUPAC Recommendations 1996)

Synopsis

The glossary contains definitions of over 270 terms frequently used in relation to the chemistry, regulation and use of pesticides. A wide range of disciplines are involved in this field and the glossary was developed as a step in facilitating communication between researchers, government regulatory authorities and chemists in associated professional areas. The range of terms includes pesticide residues, sampling for analysis, good laboratory practice, metabolism, environmental fate, effects on ecosystem, computer simulation models, toxicology and risk evaluation.

*This Report was prepared for publication by Patrick T. Holland (HortResearch Institute of New Zealand Ltd, Private Bag 3123, Hamilton, New Zealand) for the Commission on Agrochemical and the Environment of the Division of Chemistry and the Environment. The full details are to be found in Pure Appl. Chem. 1996, **68**, 1167–1193.*

Conferences

7th International Conference on Multiphoton Processes (ICOMP VII), Garmisch-Partenkirchen, Germany, 30 September— 4 October 1996

IUPAC SPONSORED

Topics to be considered include, but will not be limited to the following:

- Multiphoton and tunnel ionization of atoms and molecules;
- Intense laser fields on atoms and molecules;
- Stabilization;
- Above threshold ionization;
- Coherent control of atomic and molecular processes;
- Multiphoton processes in molecules and Coulomb explosion;
- High order generation and XUV radiation processes;
- Ultrashort laser pulse effects on atoms and molecules;
- Relativistic effects in strong radiation fields;
- Multiphoton processes in clusters and macromolecules, and on surfaces.

The conference will take place at the Congress Centre in Garmisch-Partenkirchen, a well known Olympic town which lies at the foot of Germany's highest mountain, the Zugspitze. Garmisch-Partenkirchen is reached by train in 90 minutes from Munich.

Garmisch-Partenkirchen.

The conference registration fee will be 500 DEM. The reduced registration fee for students is 150 DEM.

Further information and the second circular may be obtained from the conference secretary: Renate Weise-McKinght, Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, D-85748 Garching, Germany. Tel.: +49 89 32905 736; Fax: +49 89 32905 200. E-mail: rwm@mpq.mpg.de
It is also possible to obtain details on the Internet at http://www.mpq.mpg.de/mpq/ICOMP-VIII.html

Workshop on Pesticides: Uses and Environmental Safety in Latin America, Sao Paulo, Brazil, 13–16 October 1996

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These IUPAC sponsored workshops, held every 4 years, are scientific events growing in importance and interest, and will later this year be held for the first time in Latin America. This is a major scientific meeting which has the full backing of the Brazilian Agencies linked to agriculture, health and environment, and scientific organizations such as SBQ, FAPESP and CNq, as well as LACPA, ANDEF and AENDA.

The goal of the workshop is to discuss and to explore the approaches of risk/benefit evaluation of pesticide use in Latin American communities. Invited speakers and demonstrations of general analytical techniques are at the core of the scientific program. The following topics will be discussed:

- Environmental risk assessment;
- Regulation trends;
- Residues;
- Analytical techniques;
- Human exposure;
- and there will be the following demonstrations:;
- Immunoassay kits;
- Environmental fate;
- Modelling;
- GLP/SOP;
- Information sources; and
- Worker exposure testing kits.

The registration fee is USD 250.

Further information may be obtained from: Cynthia Bergamin, Departamento de Eventos da Sociedade Brasileira de Química, Caixa Postal 26.037, CEP: 05599-970, Brazil. Tel.: +55 (011) 210 2299; Fax: +55 (011) 814 3602; E-mail: sbqsp@quim.iq.usp.br

XXXII International Conference on Coordination Chemistry (XXXII ICCC), Santiago, Chile, 24–29 August 1997

IUPAC
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The conference will seek to cover all aspects of coordination chemistry. However, special attention will be given to those fields which are currently attracting scientists' interest, including the following:

- Theory and spectroscopy;
- Electrochemistry;
- Photochemistry;
- Macrocyclics and supramolecular structures;
- Bioinorganic;
- Organometallics;
- Catalysis;
- Materials;
- Lanthanides; and
- Education.

There will be five plenary lectures and about 20 session lectures, to cover the various fields of coordination chemistry. Besides these formal presentations, there will be minisymposia in which specific subjects will be discussed by invited speakers.

The registration fee is: USD 365 for a full participant, if paid before 31 May 1997, USD 415 if paid after 31 May 1996; USD 150 for a student, if paid before 31 May 1997, USD 200 if paid after 31 May 1997; and USD 100 for an accompanying person if paid before 31 May 1997, USD 125 if paid after 31 May 1997.

For further information, please contact: Prof. Dr Juan Costamagna, Chairman, XXXII–ICCC, Departamento de Química, Facultad de Ciencia, Universidad de Santiago de Chile, Casilla 307, Santiago-2, Chile. Tel.: +56 (562) 681 1644; Fax: +56 (562) 681 2108; E-mail: jcostama@lauca.usach.cl

13th International Symposium on Plasma Chemistry (ISPC-13), Beijing, China, 18–22 August 1997

IUPAC
SPONSORED

The International Symposium on Plasma Chemistry is the main biennual international plasma chemistry symposium, encompassing the whole of plasma chemistry including near-equilibrium thermal plasmas as well as nonequilibrium plasma. Topics will range from the basic chemistry and physics of plasmas to industrial processes and technology. International exchange of information and ideas between basic/applied researchers and practitioners of plasma processing technology will in this way be facilitated.

As with previous symposia, the 13th symposium will be preceded by a 2-day summer school on plasma chemistry and followed by a 1-day workshop on industrial applications. An exhibition of industrial equipment

will be held concurrently with the symposium.

The symposium will consist of plenary lectures, parallel oral sessions of invited and contributed papers together with poster sessions.

Topics to be covered:

Basic research

- Physical and chemical processes in plasmas;
- Modelling of plasmas and processes;
- Diagnostics of plasmas and processes; and
- Interaction of plasmas with matter.

Applied research

- Plasma processing of surfaces and materials;
- Plasma synthesis;
- Plasma coating technology;
- Plasma metallurgy;
- Plasma treatment of wastes for environmental protection;
- Plasma sources; and
- Industrial applications of plasma chemistry.

The registration fee for a participant is USD 350 for the symposium and USD 150 for the Workshop (USD 450 for both); for students the registration is USD 175 for the symposium and USD 100 for the Workshop (USD 225 for both). For an accompanying person the registration fee is USD 45.

For further information, please contact: Dr Lin He, Secretary, ISPC-13, The Chinese Society of Theoretical and Applied Mechanics, 15 Zhong Guan Cun Road, Beijing 100080, China. Fax: +86 10 62559588; E-mail: cstam@sun.ihep.ac.cn

38th Microsymposium of the Prague Meetings on Macromolecules: Recycling of Polymers, Prague, Czech Republic, 14–17 July 1997

IUPAC SPONSORED

This microsymposium is addressed to experts from academia and industry interested in assessing the present state, and future trends, in the field of plastics' waste management. This meeting aims to cover a range of approaches to possible solutions to the plastics' waste problem, with special emphasis on current intensive activity in polymer recycling. Its primary objective is to provide an interdisciplinary platform for discussions concerning environmental degradation of plastics, ways of minimizing waste generation, measures to stimulate reuse and recycling of polymers, and characterization and long-term properties of recyclates, as part of a strategy to exploit new and cost-effective secondary raw materials.

Topics to be discussed:

- Strategies for recycling;
- New processes and new concepts of recycling;
- Properties and uses of recycled polymers; and
- Environmental impact of polymers.

A plenary discussion on the future of polymer recycling will be organized.

For further information, please contact: PMM Secretariat, c/o Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, 162 06 Prague, Czech Republic, Tel.: +42 2360341; Fax: +42 2367981; E-mail: sympo@imc.cas.cz

Prague Meetings on Macromolecules—17th Discussion Conference: Surface and Interfacial Phenomena in Macromolecular Systems, Prague, Czech Republic, 21–24 July 1997

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This Discussion Conference is intended to be an open forum for both academic and industrial experts, presenting and discussing recent developments and new concepts in the field of surface and interfacial phenomena in macromolecular systems. The emphasis will be put on the behaviour of polymer chains in surface and interfacial layers, the methods used to investigate these layers in polymer systems, and the influence of interfacial phenomena on the properties of multiphase polymer blends. The discussion will also focus on identifying new trends and prospects in polymer science.

Topics to be discussed:

- Behaviour of polymer chains in surface and interfacial layers;
- Properties and methods of investigating surface and interface layers in polymers; and
- Influence of interfacial phenomena on macroscopic properties of multiphase polymer blends.

IUPAC colleagues deceased

Germany: Dr H.-J. Grosse (19 January 1996)—Commission on Atmospheric Chemistry (1986–).

Russia: Prof. K. I. Zamaraev (26 June 1996)—President of IUPAC (1994–1995), Bureau (1989–1993), President of Physical Chemistry Division (1987–1989), Committee on Publications (1990–1993), Editorial Advisory Board–Monographs on Chemistry for 21st Century (1990–1993).

Prof. K. I. Zamaraev

It is hoped to organize two panel discussions: *The Influence of Polymer Surface and Interfaces on Behaviour of Multicomponent Polymer Systems*, with G.P. Hellmann (Deutsches Kunstsoff-Institut, Darmstadt, Germany) as discussion leader, and *New Trends in the Study of Polymer Surfaces and Interfaces*, with A.R. Khokhlov (Moscow State University, Moscow, Russia) as discussion leader.

For further information, please contact: PMM Secretariat, c/o Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, 162 06 Prague, Czech Republic, Tel.: +42 2360341; Fax: +42 2367981; E-mail: sympo@imc.cas.cz

STRATEGIC RESEARCH INSTITUTE

3rd Annual Drug Discovery via Combinatorial Chemistry and Structure-Based Design, Hotel President Wilson, Geneva, Switzerland, 3–4 October 1997

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To register, or for more information, please contact the organizer: Mark Alexay, Strategic Research Institute, Tel.: +1 212 3021800 ext. 251; Fax: +1 212 3029855; E-mail: info@srinstitute.com and refer to the conference code DRP99M

Conference Calendar

1996

Environmental biotechnology

1–4 September
International Conference on Environmental Biotechnology. Palmerston North, New Zealand.
Conference Secretary, Environmental Biotechnology Conference, Process & Environmental Technology Department, Massey University, Palmerston North, New Zealand. Tel.: +64 (6) 3566254; Fax: +64 (6) 3505654. E-mail: j.c.dickson@mail.massey.ac.nz

CHEMRAWN IX

1–6 September
Sustainable Production, Use, Disposal and Recycling of Materials. Seoul, Korea.
Secretariat, IUPAC CHEMRAWN IX, c/o The Korean Chemical Society, #703, The Korea Science and Technology Centre, 635-4, Yeogsam-Dong, Kangnam-Gu, Seoul 135-703, Korea. Tel.: +82 (2) 34534019; Fax: +82 (2) 5696673.

Euroanalysis IX

1–7 September
Euroanaysis IX. Bologna, Italy.
Prof. L. Sabbatini, Dipartimento di Chimica, Università di Bari, Via Orabona 4, 70126 Bari, Italy. Tel.: +39 (80) 5442020/16/14; Fax: +39 (80) 5442026.

Medicinal chemistry

8–12 September
14th International Symposium on Medicinal Chemistry. Maastricht, Netherlands.
Van Namen & Westerlaken Congress Organization Services, PO Box 1558, 6501 BN Nijmegen, the Netherlands. Tel.: +31 (24) 3234471; Fax +31 (24) 3601159.

Food packaging

11–13 September
International symposium on Food Packaging: Ensuring Safety and Quality of Foods. Budapest, Hungary.
Dr Laura Contor—ILSI Europe, Avenue E. Mounier, 83- Box 6, B-1200 Brussels, Belgium. Tel.: +32 (2) 7710014; Fax: +32 (2) 7620014

Characterization of porous solids

15–18 September
4th International Symposium on Characterization of Porous Solids (COPS-IV). Bath, UK.
Elaine Wellingham, Conference Secretariat, Field End House, Bude Close, Nailsea, Bristol, BS19 2FQ, UK. Tel. and Fax: +44 (1275) 853311.

Chemistry of natural products

15–20 September
20th IUPAC Symposium on the Chemistry of Natural Products. Chicago, USA.
IUPAC Symposium Headquarters, 5999 Butterfield Road, Hillside, Chicago, Illinois 60161, USA. For further details, see http://www.a2z.com/iupac20/index.html

Multiphoton processes

30 September–4 October
7th International Conference on Multiphoton Processes. Garmisch Partenkirchen, Germany.
ICOMP VII Secretariat, Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, D-85748

Garching, Germany. Tel.: +49 (89) 32905736; Fax: +49 (89) 32905200. E-mail: rwm@mpq.mpg.de

Step growth polymerization

End-September
International Symposium on Step Growth Polymerization, Related Processes and Materials. Paris, France.
Dr B. Sillion, Laboratoire de Chimie Macromoléculaire, Université Pierre et Marie Curie, 4 place Jussieu, 75252 Paris Cédex 05, France. Tel.: +33 (1) 78022078; Fax: +33 (1) 78022010

Pesticide use and environmental safety

13–16 October
International Workshop 'Pesticide Use and Environmental Safety in Latin America'. Sao Paulo, Brazil.
Cynthia Bergamin, Departamento de Eventos da Sociedade Brasileira de Química, Caixa Postal 26.037, CEP: 05599–970, Brazil. Tel.: +55 (11) 2102299; Fax: +55 (11) 8143602. E-mail: sbqsp@quim.iq.usp.br

1997

Thermodynamics

5–8 January
International Symposium on Chemical and Biological Thermodynamics. Amritsar, India.
Prof. Bhajan Singh, Department of Chemistry, Guru Nanak Dev University, Amritsar–143005, India. Tel.: +91 (183) 258845; Fax: +91 (183) 258820. E-mail: bhajan@gndu.ernet.in

Recycling

4–7 February
International Recycling Congress (R'97). Geneva, Switzerland.
Dr A. Barrage, c/o LPM Limited, Tannenweg 10, CH-5712 Beinwil, Switzerland. Tel.: +41 (62) 7715555; Fax +41 (62) 7715564.

Safety in chemical production

13–17 April
3rd IUPAC Workshop on Safety in Chemical Production: Environmentally sustainable Manufacture of Competitive Products. San Francisco, USA.
Dr A. M. Ford, Gulf Coast Hazardous Substance Research Centre, Lamar University, PO Box 10613, Beaumont, Texas 77710-0613, USA. Tel.: +1 409 880 8768; Fax: +1 409 880 2397.

Bioorganic chemistry

1–6 June
4th International Symposium on Bioorganic Chemistry. Biarritz, France.
Prof. A. Marquet, Université Paris URA CNRS 493, Laboratoire de Chimie Organique Biologique, Tour 44/45-4 Pl. Jussieu, 75252 Paris Cedex 05, France.

Recycling of polymers

14–17 July
38th Microsymposium on Macromolecules, Recycling of Polymers. Prague, Czech Republic.
P.M.M. Secretariat, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám 2, 162 06 Prague c-Petriny, Czech Republic. Tel.: +42 (2) 360341; Fax: +42 (2) 367891. E-.nail: sympo@imc.cas.cz

Interfacial phenomena

21–24 July
17th Discussion Conference on Macromolecules, Surface and Interfacial Phenomena in Macromolecular Systems. Prague, Czech Republic.
P.M.M. Secretariat, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám 2, 162 06 Prague c-Petriny, Czech Republic. Tel.: +42 (2) 360341; Fax: +42 (2) 367891. E-mail: sympo@imc.cas.cz

Bioinorganic chemistry

27 July–1 August
8th International Conference on Bioinorganic Chemistry. Yokohama, Japan.
Prof. M. Hidai, Department of Chemistry & Biotechnology, Graduate School of Engineering, The University of Tokyo, Hongo, Tokyo, Japan

Plasma chemistry

18–22 August
13th International Symposium on Plasma Chemistry. Beijing, China.
Dr Lin He, The Chinese Society of Theoretical & Applied Mechanics, 15 Zhong Guan Cun Road, Beijing 100080, China

IUPAC Congress

18–22 August
36th IUPAC Congress. Geneva, Switzerland.
36th IUPAC '97, c/o AKM Congress Service, PO Box 37, CH-1218 Le Grand-Saconnex/GE, Switzerland. Tel.: +41 (22) 7611661; Fax: +41 (22) 7611662.

IUPAC General Assembly

23–30 August
39th IUPAC General Assembly. Geneva, Switzerland.
The IUPAC General Assembly is not open for general participation but restricted to members of IUPAC bodies that meet on this occasion.

Coordination chemistry

24–29 August
32nd International Conference on Coordination Chemistry. Santiago, Chile.
Prof. J. Costamagna, Departamento de Química, Facultad de Ciencia, Universidad de Santiago di Chile, Casilla 307, Santiago-2, Chile. Tel.: +56 (2) 6811644; Fax: +56 (2) 6812108. E-mail: jcostama@lauca.usach.cl

Spectroscopicum internationale

21–26 September
30th Colloquium Spectroscopicum Internationale 1997 (CSI). Melbourne, Australia.
The Meeting Planners, 108 Church Street, Hawthorn Victoria 3122, Australia. Tel.: +61 (3) 98193700; Fax: +61 (3) 98195978.

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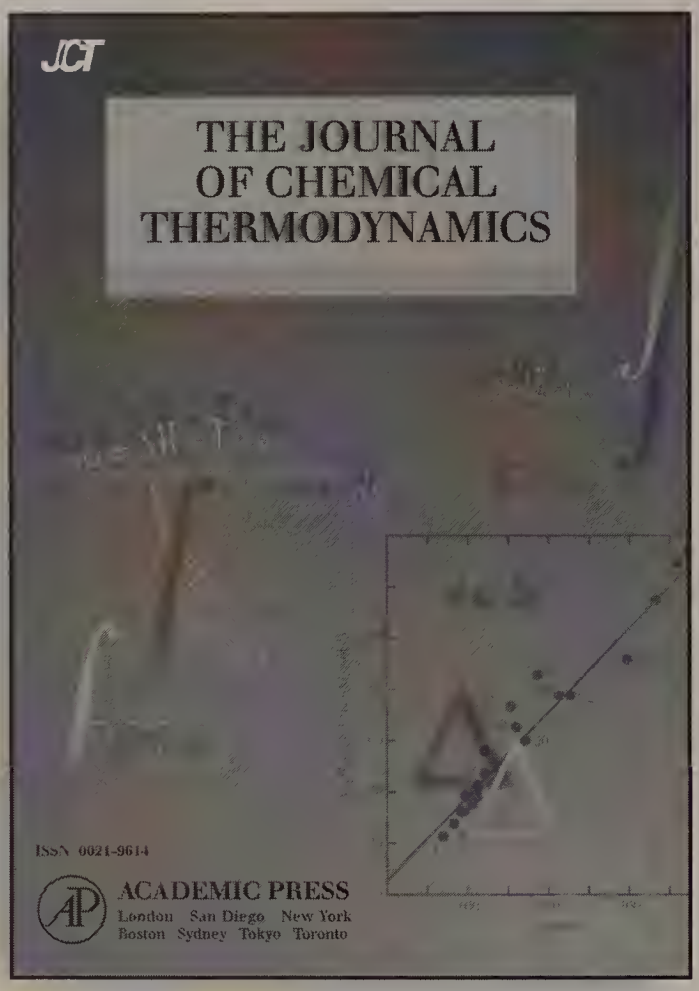

The Journal of Chemical Thermodynamics has established itself as the premier vehicle for the dissemination of the results of research in chemical thermodynamics. The reputation of the Journal is due in large measure to the efforts of Professor Max L. McGlashan who has served as editor for 27 years and retired from active editorial duty with the last issue of 1995.

In 1996 the Journal has seen some changes: a new cover and an expansion of the scope of articles accepted for publication. The articles accepted may now encompass areas such as:

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-interfaces
-high temperature chemistry

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The International Union of Pure and Applied Chemistry (IUPAC), formed in 1919, is a voluntary non-governmental, non-profit association of organizations, each of which represents the chemists of a member country.

Its objectives are:

- to promote continuing co-operation among the chemists of the member countries;
- to study topics of international importance to pure and applied chemistry which need regulation, standardization, or codification;
- to co-operate with other international organizations which deal with topics of a chemical nature;
- to contribute to the advancement of pure and applied chemistry in all its aspects.

The membership of IUPAC presently comprises 40 countries, each represented by a national organization, such as an academy of science or research council.

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Chemistry International

IUPAC

1996, Vol. 18, No. 5 (September)

201 Secretary General's Column
Edwin D. Becker

203 International Organization for Standardization

205 PAC Review

209 Commission and Committee news

213 The Thieme–IUPAC Prize

214 News

220 New Publications

225 Recent Reports

226 Conferences

229 Conference Calendar

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Front cover: Brisbane.

Brisbane '96

The 14th International Conference on Chemical Education (ICCE)—Chemistry: Expanding the Boundaries

The 14th International Conference on Chemical Education was held on the campus of the University of Queensland, Brisbane, Australia, from the 14th to the 19th of July, 1996. Brisbane is the capital city of the State of Queensland, Australia, which is situated in the sub-tropics on the edge of the Asia Pacific rim. The city is the central hub for visiting Queensland, the most popular tourist state in Australia, it is close to the Gold and Sunshine Coasts and within easy reach of the Great Barrier Reef, the world heritage site of Fraser Island, the rain forest hinterlands of the surrounding mountains and the outback beyond.

The campus of the University of Queensland occupies a bend in the meandering Brisbane River. The campus is green and beautifully laid out. There are numerous small lakes which are full—to the eyes and ears of a European correspondent—of exotic birds whose songs were a delight. During the conference the weather was bright and sunny—Antipodean winter days which were as warm as a British summer.

The conference was well attended with over 500 registrants in addition to school and day registrants. Chemical educators from all over the world had made the journey to Brisbane for this, the 14th in a very successful series of conferences. There were attendees from as far away as Scotland and even some from Papua New-Guinea. In detail, there were 64 participants from the United States, 19 from Japan, 23 from Africa, 40 from the European Union with 5 from Eastern Europe. On any one day there might be up to 80 day participants from local schools and colleges with 169 Australian full registrants.

The conference was divided up into Plenary Lectures, which were held first thing each morning. These full lectures would be followed by smaller parallel Symposia which would address a wide variety of subjects. In the afternoons there would be parallel Keynote Lectures and Workshops. The following descriptions give a flavour of the type of material presented and discussed during this meeting.

Fig. 1 Brisbane, a city in the sub-tropics.

Plenary lectures

Investigating chemical dynamics by laser and molecular beam techniques

Yuan Tseh Lee, Nobel Laureate (Academia Sinica, Taipei, Taiwan)

Chemistry is the study of material transformations. Yet a knowledge of the rate, or time dependence, of chemical change is of critical importance for the successful synthesis of new materials and for the utilization of the energy generated by a chemical reaction. During the past century it has become clear that all macroscopic chemical processes consist of many elementary chemical reactions that are themselves simply a series of encounters between atomic or molecular species. In order to understand the time-dependence of chemical reactions, chemical kineticists have traditionally focused on sorting out all of the elementary chemical reactions involved in a macroscopic chemical process and determining their respective rates.

During the past three decades, with the development of many sophisticated experimental techniques, it has become possible to study the dynamics of elementary chemical reactions in the laboratory. For example, detailed information on the nascent quantum state distributions of simple products for some chemical reactions can be derived from the chemiluminescence spectra of reaction products obtained under single collision conditions, the analysis of the threshold operating conditions of a chemical laser, or the spectra obtained using various linear or nonlinear laser spectroscopic techniques.

As might be imagined, Prof. Lee is a most accomplished speaker. His talk was a perfect demonstration of how to present to a mixed audience (a variety of different types of chemists of differing levels of specialization) a complex topic at the forefront of fundamental research, but a topic of great interest and importance—as befits a conference on chemical education.

Prof. Lee began by discussing a simple combustion reaction

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

which although strongly exothermic, needed initiation. A consideration of this deceptively simple reaction led to a discussion of the Arrhenius rate equation and an explanation of what the two terms in this equation, the pre-exponential cross-section factor and the activation energy, mean with respect to simple chemical reactions. How, for example, in the low temperature combustion of methane, the reaction

$$CO + OH \rightarrow CO_2 + H$$

is of considerable importance. However, this reaction has been observed only to proceed when there is an appropriately orientated collision between the reactants—the oxygen of the OH must approach the carbon end of the carbon monoxide molecule for the reaction to proceed.

After this example of how the rate of a chemical process may be influenced by orienting the interacting molecule, Prof. Lee considered how the rate of reaction might be increased by varying the energy content of the reactants. For example, in a reaction such as

$$F + D_2 \rightarrow DF + D$$

a study of where the energy released by the reaction is to be found in the products—which vibrational and rotational states of the DF product are populated—allows one to predict how best to place energy in the reactants to push the reverse reaction.

The remainder of Prof. Lee's fascinating talk covered his recent research into mode-selective chemistry. He considered the reactions

$$H_2S \rightarrow H_2 + S$$

and

$$H_2S \rightarrow HS + H$$

and how these reactions might be forced by using a multiphoton absorption of H_2S to drive the decomposition. For example, if the energy required to decompose the reactant was placed in the H_2S molecule by strongly exciting the bending motion, then the mechanics of the bending process, at high amplitude, would bring the two hydrogen atoms closer together. Likewise, if the energy necessary to drive the reaction was added by exciting the asymmetric stretch of the H_2S molecule, then one hydrogen atom would be driven towards the S atom and one would be driven away from the S atom. Prof. Lee explained his results with very simple and memorable images.

It is likely that these experiments will lead to a rapid rise of interest in this field, which could well be set to fundamentally change our picture of chemical reactivity. Most chemistry is done by 'shaking and baking'—one mixes the reactants, heats the system, and extracts the products. In many cases, heat is produced which may push a reaction along several different paths at the same time—one that produces the desired product, and others, perhaps the majority, which produce nothing of interest. However, if it becomes possible to nudge the chemical reactivity of particular bonds in a molecule, the reactants might well follow only a limited number of pathways, thereby eliminating waste and the possible production of unwanted products.

Is there a set of competencies for a graduating chemist?

David Gardiner (Queensland University of Technology, Australia), Martin Bridgestock (Griffith University, Australia), Joe Baker (Commissioner for the Environment, Canberra, Australia), Gary Golding (Queensland Government Chemical Laboratories, Brisbane, Australia), Greg Kilmister (Australian Laboratory Services, Brisbane, Australia), Edelene Wintrup-Byrne (Queensland University of Technology, Brisbane, Australia), Vanessa Masters (The University of Queensland, Brisbane, Australia).

This Plenary session was given over to a panel discussion about what a graduating chemist should know. The panel was composed of university teachers and industrialists, together with a recently graduated chemist and an expert on scientific ethics.

It was interesting to learn that both industrialists—both from laboratories which undertake chemical analysis on a commercial basis—stressed that they would prefer if students came to them better equipped to deal with problems of health and safety at work, together with an understanding of ISO standards and Quality Assurance. The university teachers protested that such topics were, at best, only taught in some universities and in the final year as optional short courses. However, it was stated that some teaching of these topics

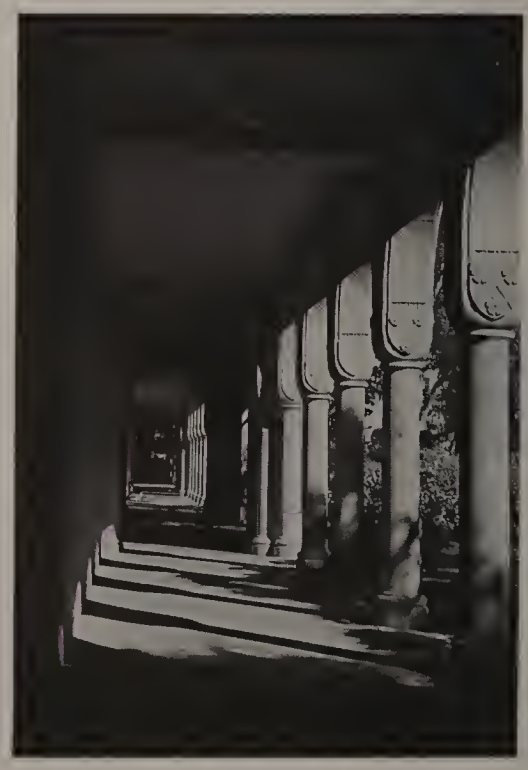


Fig. 2 The imitation Romanesque cloister on the campus of the University of Queensland.

was set to become mandatory throughout the university system in Australia. Not surprisingly, the expert on ethics insisted that graduating science students should all have a grounding in what ethics was all about and how this awareness was important for the role of the scientists in society. However, as was pointed out—there are only so many teaching weeks in an academic year.

The air we breathe

Mike Pilling (School of Chemistry, University of Leeds, Leeds, UK)

The need for a better understanding of the chemical and physical processes affecting air quality provides a major impetus in atmospheric science. Health impacts are a central concern through their effect on the quality of life, while new legislation brings with it inevitable financial burdens. Together these provide an increasing driving force and a justification for new work on modelling and monitoring of the atmosphere, coupled with underpinning laboratory experiments. Recent work in all of these areas were presented to illustrate current studies or urban air quality.

The mechanisms of chemical processes occurring at short timescales, linking NO, NO_2 and O_3, and on longer timescales leading to photochemical smog, were discussed, together with ways in which the kinetics of individual reactions can be studied in the laboratory using laser techniques and important species monitored in the field.

Prof. Pilling described an experimental programme he has established in Leeds (UK) which monitors the concentration of a variety of the radicals, important in atmospheric chemistry, present in the ocean winds blowing ashore on the west coast of Ireland.

Nuclear energy: a solution to greenhouse gases

Ian Lowe (Griffith University, Brisbane, Australia) and Ian Hore-Lacy (Uranium Information Centre, Melbourne, Australia)

In the last 40 years, we have seen nuclear energy take its place as a major source of electricity world-wide. It now produces 17% of the world's electricity and could conceivably produce a higher proportion, to displace some 6 billion tonnes of carbon dioxide emissions per year. Concerns about global warming and environmental quality now underline the virtues of nuclear electricity among other sources of energy.

This Plenary Lecture was given over to a debate on the use of nuclear power. It was first pointed out that today, nuclear energy is a mature technology. Over 1200 nuclear reactors have been built and operated, some of these have been decommissioned and among

Fig. 3 Opening ceremony of the 14th ICCE (Photograph courtesy of Ms Jelena Edhouse).

the 430 reactors in commercial operation the first advanced reactors are now entering service. This debate examined issues affecting the public acceptability of nuclear energy, including its role in burning material liberated from nuclear weapons stockpiles and the management of high-level wastes.

Chemistry at the interface of history and art

Mary Virginia Orna (Department of Chemistry, College of New Rochelle, New Rochelle, USA)

The methods of modern chemistry can be used as probes to examine the origins and to aid in the conservation of art objects and artefacts of historical interest. In addition, these methods can help to clarify the techniques by which these objects were made and the nature of the naturally occurring and synthetic materials used. A variety of instrumental methods illustrated in the examination of such materials as medieval manuscripts, 20th century art forgeries, the Vinland Map and the Shroud of Turin. Although such methods can give great insight into the objects in question, there are limits to such technology; these limitations were also discussed.

Symposia

The Importance of imagery in chemistry

Organizer: Robert Bucat (Department of Chemistry, The University of Western Australia, Nedlands, 3907, Western Australia)

Imagination, which is different from memory, is a central component of scientific progress. An important component of imagination is imagery; that is, the forming of pictures in the mind to aid in the understanding of a particular concept. The story of Kékule's 'dreams' of monkeys holding bananas while trying to understand the structure of benzene is probably the most famous

example. Likewise, Rutherford created a powerful image to account for the results of his a-ray scattering by thin metal foils, and gave us his remarkable picture of the atom with the first ideas about the nature of the heavy nucleus. Understanding kinetic theory explanations of gas behaviour is not possible without mind pictures of particles dashing rapidly through space. Kinetic molecular theory is inconceivable as an explanation of behaviour unless one accepts that matter is particulate—a picture that some of the world's foremost scientists found impossible to imagine for decades, even after Dalton.

In this symposium, the speakers took for granted the view that learning chemistry involves, amongst other things, students making sense of macroscopic observables at the sub-microscopic level, and that this demands rich mental images. The speakers questioned whether the significance of the role of imagery in sense-making for students is generally appreciated. A perusal of textbooks suggests that it is not. The symposium considered the images that are essential for sense-making in selected chemistry topics and the consequent implications for the teaching of these topics. Attention was also paid to the quality of these mental images and how inappropriate images might well be contributing factors in many of the student 'misconceptions' that have been identified over the past decade or two.

The four presentations comprising this symposium were reflections borne out of research studies in the classroom at either secondary or tertiary levels, on the importance of imagery in four widely different chemical contexts. Do we perhaps too often ignore imagery and modelling in favour of algorithmic mathematical manipulations? Yes we do, according to John Oversby (University of Reading, UK). While focusing on the topic of acidity in aqueous solutions, Dr Overby argued that in a number of areas of chemistry, we would do well to concentrate more on the development of appropriate models or mind pictures. He believes that the investment in acquiring such models has a payoff in the form of rendering the related mathematics more meaningful to the student.

Ruth Ben-Zvi (Weizmann Institute of Science, Israel) argued that interpretation of many of the chemical concepts that we commonly use (such as the equations that we use to represent chemical reactions) can be more profound for students than we sometimes realize. Understanding chemical concepts in the way that chemists do involves perhaps a surprising complexity of imagery. Ms. Ben-Zvi addressed the difficulties of achieving this level of imagery, as well as the implications of incorrect or inadequate images.

As an example, Ms. Ben-Zvi chose to discuss how one teaches students about entropy. She showed some pages from standard textbooks which invariably define entropy mathematically or in terms of concepts which many students would find difficult to comprehend or relate to. However, when she spoke about a hypothetical student who arrives home and dropped his/her bag in one part of a room, his/her coat in another part of the room, and leaves their shoes somewhere else, then that person is increasing the entropy of the universe and this image gives the teacher a starting point from which to begin a discussion of entropy. As Ms. Ben-Zvi pointed out, those students who are keen to learn do not really need teachers, they will work it out for themselves and read the appropriate texts. But teachers are now more cognisant that more effort needs to be spent on the less keen students, and images—even if somewhat exagerated—do have an important role in teaching.

School teacher Jaya Chowdhury (Pen Rhos College, Western Australia) is involved in research towards a PhD degree. She is trying to understand the difficulties that her students in lower secondary school experience in writing chemical equations. Recognizing that the most fundamental step is visualization of what species are involved in a chemical reaction, Ms. Chowdhury analysed the demands placed on students in order to visualize the species represented by a range of formulas in common use at this level of schooling. As the chairman of the session pointed out when introducing Ms Chowdhury, 'only teachers made of steel will want to hear what this analysis reveals.'

Janette Head (University of Western Australia) and Bob Bucat reported on Ms Head's findings from an investigation into university students' abilities in common stereochemistry tasks—of the sort that are necessary to make sense of diagrams that chemistry educators commonly use. She has found considerable differences in their abilities to perform mental manipulations of the three dimensional images that correspond with two dimensional diagrams. More fascinating are the differences in the strategies that they use for tasks that require a comparison of the structures represented by two diagrams. Her findings present enormous challenges to lecturers, given that amongst a student audience there may be a number of preferred strategies for tackling a given task, only one of which corresponds with that described by the lecturer.

Nobel Laureate Yuan Tseh Lee presented undeniable arguments concerning the vital role of imagery in his research as he gathers experimental evidence to assist in visualization of the critical moment when molecules collide and react. Just as researchers commonly translate between imagined events at the molecular level and observable behaviour, so too students of chemistry are required to make microscopic/macroscopic mental transitions for sense-making. It is important that these transitions are well grounded in science and explained by teachers.

The independent learner and distance education

Organizer: Stuart W Bennett (Faculty of Science, Open University, Milton Keynes, United Kingdom)

Practitioners of distance education in chemistry have had to address a range of problems which include limited access of students to teachers, access to information sources such as libraries, and restrictions in laboratory work. Many creative and ingenious approaches have been devised which today have a wide applicability. Almost everyone involved in tertiary and secondary chemistry education is facing the challenge of providing a high quality education for increasing numbers of students with limited resource. The experiences of distance learning can provide the means to address this problem. This Symposium comprised presentations from four speakers and included a discussion period with contributions from the audience.

Prof. Casper Schutte (University of South Africa) focused on the role of the text book in the next decade. Not only is it likely that the paper text will gradually disappear and be replaced by an electronic-access medium, but the capability and use-mode will undergo a revolution. The interactive 'text' will allow alternative learning routes, provide database interrogation, and rapid communication between learner and teacher, who may well be separated by substantial distances. The distinction (and relative advantages) of the campus-based learner compared with the distance learner will disappear in a very few years.

Prof. Schutte pointed out that in the 1960s it was perceived that television would replace the traditional university teacher. This did not happen, even though the Open University in the UK has been a tremendous success. However, the Internet and modern developments in computer technology make a future fundamental change in the method of teaching inevitable. It was pointed out that with the speed of modern personal computers and the accessibility of databases, individuals can search such databases in real time. The World Wide Web (WWW) allows one to access huge quantities of data anywhere. For example, the use of the quantum chemistry package GAUSSIAN on a personal computer would allow a student to perform *ab initio* calculation on molecular structure, the results of which could then be compared with data held in the appropriate database. Such scenarios would, according to Prof. Schutte, allow us to re-plan the teaching of chemistry.

In this brave new world of chemistry teaching it would not even be necessary for the teacher and the student to be in the same room. Indeed, they need not be in the same country. The teacher would pose a question—a dialogue process—which the student would seek to answer by exploring the Internet and in so doing educate himself.

The practical aspect of chemistry is one area where alternatives to 'hands on' experience are less easy to find. The Open University in the UK has been successfully providing education in chemistry through distance learning for 15 years through a multi-pronged attack on practical work. Dr Stuart Bennett has developed a programme for the progressive development of practical skills through alternative media which include non-returnable home experiment kits, multimedia methods and experiment design theory. The prescription and assessment of the achievement of behavioural objectives forms an essential part of this approach.

Dr Bennett pointed out that setting up and running laboratory classes is very expensive. The current insistence on increased health and safety at work is continuing to push up the costs of running chemical laboratories. Indeed, he cited an example of a laboratory in the US where the biggest single item on the budget of the laboratory was the correct legal disposal of waste chemicals. Against this background, chemistry must continue to be taught. However, one should redesign practical chemistry courses to develop particular skills in students. Dr Bennett showed how some laboratory skills could be developed outside the laboratory, via electronic interactive communications, and in this way save time and resources in the laboratory. As examples of these laboratory skills which could be learned outside the laboratory, Dr Bennett discussed: data generation, data analysis, report writing, decision making and design of apparatus, and signal-to-noise calculations.

All too often, new ideas about chemical education are put into practice, but performance is inadequately assessed. The programme developed by Drs Ma Christina Padolina and Marcelita Magno in the Philippines, for the distance training of secondary school teachers, provides a solution to the need for continuing in-service training. Follow-up research has identified factors (of both a structural and personal nature) that

Fig. 4 Participants of one of the small Symposia held during the 14th ICCE (Photograph courtesy of Ms Jelena Edhouse).

are influential on the training outcomes. Their presentation explored techniques for the assessment of outcomes that may be applied to all such programmes.

Should and can 'real' chemistry be taught to elementary students?

Organizer: Keith Skamp, Associate Professor (Southern Cross University, Lismore NSW, Australia)

This symposium addressed the issue of what type of content is suitable in elementary science. In particular, it asked if elementary students (5–13-year-olds) can learn chemistry, and if so how can it be taught most effectively? 'Real' chemistry is open to interpretation, but is meant to at least partially imply whether young learners can appreciate ideas related to, for example, atoms and molecules, the periodic table, acids and bases and the behaviour of chemical substances. The four speakers and the organizer presented case studies of projects and lesson sequences which responded to the symposium title in the affirmative. They also confronted the question of whether such topics are too abstract or irrelevant to young learners. There was an opportunity to raise issues with the presenters and debate the symposium topic. The speakers were classroom practitioners and university teachers.

Carolyn Potts (Buchanan Elementary, Livonia, Michigan, USA) provided an overview of a 5-week module for sixth grade students which focused on a hands-on, investigative approach to mass vs. volume, structure of the atom, the periodic table, elements and compounds, acids and bases, physical and chemical properties and changes. Exemplar activities were mentioned which provided students with the opportunity to collect, analyse and verify data and practice problem-solving skills. Examples of extracts from the students' journals were presented which highlight their thoughts on the investigative process. These journals have been published by the school district.

Marion Davies (Edgewood College of Education, Ashley, Natal, South Africa) described the type of chemistry introduced into some elementary schools in South Africa. Reference was made to the apparatus which is being used (especially in the poorer schools). The feasibility of introducing topics such as the 'particulate nature of matter' were discussed, and how it is needed to explain certain concepts (e.g. phase change). Other topics thought suitable for the elementary school were discussed: solubility and the concepts of hard and soft water, and aspects of the periodic table.

Lynn Hogue (Miami University, Middleton, OH, USA) argued that real chemistry can only be taught to young learners if the chemical concepts are connected to everyday experiences and observable phenomena. Her work at the Centre for Chemical Education has been involved with teacher enhancement programming for elementary teachers, which has incorporated the development and testing of numerous 'real' chemistry activities for elementary students. Two-way innovative links have been made with the world of children through two programmes, one using toys as scientific tools and the other integrating science and children's literature. Activities from each programme (which meet National guidelines, e.g. Benchmarks for Science Literacy) were discussed, as well as the results of an outside evaluation confirming that the methods used are improving elementary science education.

Learning through visualization of the molecular level

Organizer: Roy F. Tasker, Senior Lecturer (Faculty of Science and Technology, University of Western Sydney, Nepean, Sydney, Australia)

A deep understanding of chemistry requires a well developed mental model of structures and processes at the molecular level. The meaning of reaction mechanisms, chemical equations, colligative properties and many other topics require a model of many molecules and ions interacting with one another. Such a model may not always be developed adequately from static textbook diagrams. Visualizing this level in dynamic images requires different degrees of artistic licence, hence great care is needed to avoid creating new misconceptions—images are powerful and memorable, the teacher should not get them wrong. Educational research has already established a link between some misconceptions and poorly presented images of the molecular world. In addition, some authors have expressed concern that the sophistication of the technology used in molecular visualization by computer simulation may not be matched with appropriate sophistication in its educational use.

Some of the questions considered in this Symposium included the following:

- Are static, two dimensional representations of the dynamic, three dimensional molecular world satisfactory mental models?
- What effect, if any, does artistic licence—such as the use of colour, collision sounds, ball and stick representations and slowed-down molecular movement—have on developing useful mental models?
- Can images of molecules and ions reacting together facilitate a deeper understanding of chemical symbolism and notation (e.g. balanced equations and stoichiometry)?
- Can the richness, information density, and visual impact of molecular animations promote new, unforeseen misconceptions that are even more resistant to change?.

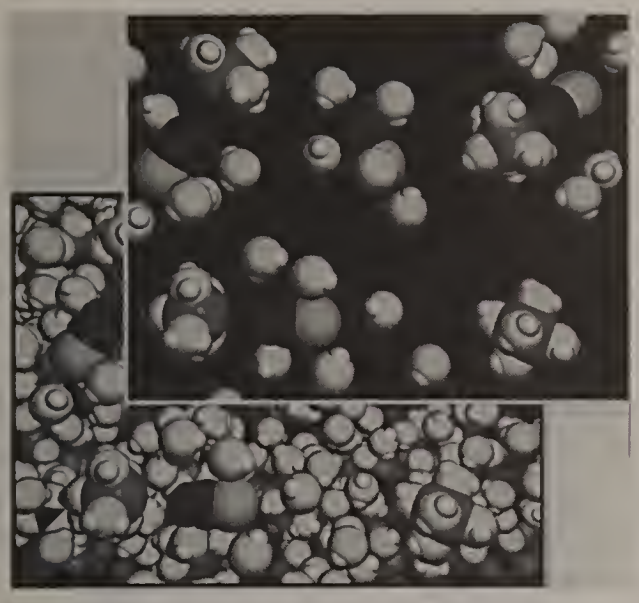


Fig. 5 An image from a VisChem simulation of an aqueous solution. (For more information about VisChem, please Email: j.field@nepean.uws.edu.au).

The Symposium consisted of four speakers each using visualization of the molecular level in different ways:

Peter Atkins (Oxford University, UK), a leading writer of textbooks and general reading books in chemistry, illustrates his work with molecular representations. He went on to consider the challenge of using these representations in the book format.

George Bodner (Purdue University, USA) described some of the techniques that can be used to help students visualize molecules so that tasks, ranging from balancing redox equations to predicting the product of a chemical reaction, can involve manipulation of particles rather than letters, lines and numbers.

Corrie du Toit (University of Potchefstroom, South Africa) described how many students are unable to visualize an oxidation reduction reaction due to a lack of images of electron configuration and changes in oxidation number.

Roy Tasker showed a selection of multi-particle, three dimensional animations produced in the VisChem project (Learning Chemistry through Visualization of the Molecular World), that portray substances and their reactions, and described their uses and evaluation. These VisChem demonstrations were truly remarkable. The first was a representation of a lattice of NaCl melting where the increasing levels of vibrational agitation were clearly seen as the temperature increased, and a lattice of NaCl dissolving in water where one could see the water molecules pulling ions out of the lattice. Likewise, redox reactions were also visualized by the VisChem project animations. Reactions such as

$$Ag^{+}_{(aq)} + NO_3^{-}{}_{(aq)} + Na^{+}_{(aq)} + Cl^{-}_{(aq)} \rightarrow AgCl_{(s)} + Na^{+}_{(aq)} + NO_3^{-}{}_{(aq)}$$

followed in an animation, clearly demonstrated the creation of a white solid from the mixing of two colourless liquids.

Keynote talks

Metal units in supramolecular structures

Jack Harrowfield (The University of Western Australia, Australia)

The human body provides a wonderfully complex example of a system which is absolutely dependent upon the presence of metals for its continued functioning, yet it can malfunction with both insufficiency and excess of essential metals, and even cease to function at all in the presence of quite small amounts of exotic metals.

These facts have provided a major stimulus for the study of metal ion (usually cation) chemistry, and such study has in turn provided means not only of controlling metal ions in biological systems but also of exploiting the properties of metal ions in general. Thus, it has been of benefit to mining as well as medicine, to ecology as well as analysis. The pathway to such benefits has been the use of special and selective metal ion binding entities or 'receptors'. However, a fundamental question to which Nature has provided but a partial answer is 'How is a selective metal ion receptor synthesized?'. In fact, one way of conducting such a synthesis is to use the particular metal ion to control the reaction. This involves the metal as a 'template', where factors such as the number of species bound to the metal, their distribution in space and the influence of the metal on their reactivity are all exploited. This notion of the metal ion function is one which is useful in analysing many other aspects of metal ion chemistry and so is the focus of the present discussion concerning chemistry ranging from the synthesis of metal cages to the properties of triple helices.

A glimmer of light amidst failures: Luminescence from polymers

Graeme A. George (School of Chemistry, QUT, Brisbane, Australia)

The emission of visible light from biological processes (bioluminescence) or from chemical reactions (chemiluminescence) has fascinated mankind. Most recently, it has been found that polymers also emit chemiluminescence—in some cases it is very weak and accompanies the oxidative degradation and mechanical failure of the polymer chain; and in other cases, it is very bright as in the recently devised light emitting polymer diode.

Both processes provide an opportunity to explore the unique properties of polymers which may in some cases be insulators undergoing free radical formation producing chemiluminescence, and in other cases, conductors generating electroluminescence with col-

ours controlled by the particular chemical structure. The opportunities for demonstrating some important features of polymer chemistry and structure, free radical reactions and electronic excited states through polymer luminescence were illustrated.

How does the ageing chemist get a date? Archaeometry

Peter Pomery (Department of Chemistry, The University of Queensland, Brisbane, Australia)

There is increasing interest of modern societies in investigating their past history and heritage. This has been seen by many as being the preserve of archaeologists and historians. However, it is becoming increasingly clear that chemistry, chemists and the scientific method have an important role to play in these investigations of history and prehistory. In this lecture, the role of chemistry in archaeology was explored in relation to determining the ages of a range of archaeological and geological materials. Many of the techniques that have been developed are derived from fundamental concepts in chemistry. They are therefore ideally suited as an introduction into the teaching of chemistry as relevant resource material as well as offering possible material for some problem-based style learning. Topics addressed included:

- How are the ages of materials determined?
- The range of dating techniques available;
- Selection of an appropriate dating technique;
- What types of materials can be dated?
- Can fakes be detected easily?
- Simple demonstrations to illustrate some methodologies.

Current work at The University of Queensland in developing a new dating technique was discussed and illustrated with a range of examples and demonstrations.

The book, the disc and the future

Peter Atkins (University of Oxford, UK)

> 'The increasingly widespread availability of multimedia promises to take us over the current pedagogical horizon. But what lies beyond: an intellectual gulch or the Garden of Eden?'

In this talk, the speaker, an eminent scientific author with at least 30 titles to his credit, looked at the promise that multimedia holds from the point of view of an author and the instructor. He discussed how multimedia extends the scope of books and how authors might use this technology. But, as well as extending our horizons, it is possible that there will be losses as the printed page gives way to the disk, and Dr Atkins explored these aspects. Regardless of its disadvantages, the future is the disk, in some form or other and the speaker examined the opportunities that it gives us to make the presentation of chemistry dynamic, involving and interactive.

Dr Atkins began by characterizing a textbook as a 'frozen fish'—an image of something that is unchanging and capable of supporting only limited interactions—indeed, of limited shelf life. Previously, a student would have read a textbook, now they have the chance to see the film of the textbook. Dr Atkins pointed out that the application of new technology to the teaching of chemistry would allow the visualization of dynamic processes in teaching. For example, with a static unchanging book, it is difficult to teach the structure of liquids, which is an inherently dynamic process.

The down-side of the application of multimedia technology to chemistry teaching is that both students and teachers must become computer literate. Also, the preparation of a multimedia package requires very different skills from the authorship of a traditional textbook—not only must the text be readable, but there has to be significant attention paid to layout and design. If multimedia methods of instruction attains even some of the popularity predicted for them, there is a danger that the human instructor will become redundant. That the computer will take over the entire instructional process with loss of jobs—a downsizing of the academic world. As stressed by the speaker, this is probably not a positive move, as the instructor fulfils many roles other than simply acting as a source of information.

This talk was certainly thought provoking, and the discussion which followed on the application of virtual reality to the design of teaching aids contained some memorable images suggested for future generations of instructional aids—'imagine being inside a lattice and listening to the phonons.'

1999 International Chemistry Celebration

During the 14th International Conference on Chemical Education, Brisbane, a meeting organized by the Committee for the International Chemistry Celebration, of the American Chemical Society (ACS) and by the Royal Australian Chemical Institute was held to consider how best to organize the International Chemistry Celebration (IChC) in 1999.

The mission of the International Chemistry Celebration 1999 is to enhance the public perception of chemistry and its contributions to everyday life throughout the world, and to reinforce communication among the various national chemical societies, and organizations involved in chemistry world-wide.

In order to accomplish this mission, the American Chemical Society will play the leadership role in establishing a global network of organizations dedicated to the promotion of the positive image of chemistry. By working together as partners and sharing information,

Chemistry Week in Australia

Going Strong Since 1982

VOLUME 2, ISSUE 2 JULY 1996

Australia was one of the first countries to initiate a National Chemistry Week program, and its wide-ranging activities have provided a useful model for newer Chemistry Weeks around the world. The Royal Australian Chemical Institute (RACI) held its first National Chemistry Week in 1982, with the goal of promoting an appreciation of the role of chemists and chemistry in society. Since the beginning, RACI members have tried to reach as many members of the community as possible. Audiences which receive special emphasis include students at the primary, secondary, and tertiary school levels, as well as members of the general public and the scientific world.

One of the highlights of each year's program is the National Chemistry Quiz. The Quiz is held at two junior levels (Years 7 and 8, and Years 9 and 10) and two senior levels (Year 11 and Year 12).

Beginning with 8,850 student participants in 1982 the Quiz has grown steadily and now attracts entries from all Australian States and from the neighboring countries of Fiji, Malaysia, New Zealand, Papua New Guinea, The Philippines, Singapore, Vietnam, and Western Samoa. The 1996 Quiz, scheduled for July 25, promises to be the most successful one yet, with over 80,000 participants from 1,200 schools.

The purpose of the Quiz is to help secondary school students develop an appreciation for the role of chemistry in society. Many Quiz questions emphasize the connection between the academic image of chemistry and its important day-to-day applications in the home, the environment, and industry. Where possible, questions are free of specific syllabus content. Once students have done the Quiz, teachers may use it as a teaching tool by going through the answers to the questions. As one student wrote, "I learned a great deal about the uses of chemistry in the real world through the questions in the paper. The Quiz has helped me to think more laterally in chemistry" In order to encourage and recognize those who take the Quiz about 40 percent of the students receive a Certificate of Merit. Awards and certificates are presented by chemists who visit the school.

Students in Australia seem to have a flair for chemistry, creativity—and competition. A number of other competitions have also become a regular part of the National Chemistry Week program.

In the National Chemical Analysis Competition, school teams compete in a titration contest at the regional level. The best teams advance to the national competition, in which they are required to determine the amount of

continued on page 2

Researchers for the National Chemistry Quiz recently presented a poster at Pyrotechnic '96 on "Factors Affecting the Performance of Students in the RACI Chemistry Quiz." From left, Chris Owens, John Beard, Charles Feglaris, and Audrey Wilson

Winners in the 1994 Chemical Analysis Competition, from Bundoran Catholic High School. From left, Tamara Lazzaris, Amber Mutter, Amanda Torkington, and Mike Clark (coach)

Fig. 6 The latest issue of the news (*NeWS*) magazine of the International Chemistry Celebration 1999 organization.

experience and resources, the members of this network will plan and carry out a series of events throughout 1999 to highlight the everyday relevance of chemistry.

The meeting in Brisbane was chaired by Dr Helen Free (ACS) and by Dr Susan Cummings (Royal Australian Chemical Institute—RACI). Many different countries were represented, and Dr Free started the meeting by talking about the need for an international celebration of chemistry. She wanted to get as many national chemical societies as possible to participate with the ACS to promote chemistry in 1999.

It was decided that the last two weeks in April 1999 would be set aside in as the most probable dates for a series of meetings/celebrations held around the world which would have a common theme—the celebration of chemistry. In 1999, IUPAC will be having a General Assembly in Berlin which will also be hosting the IUPAC Congress. So IUPAC will be making its contribution to the chemistry celebrations in 1999

Copies of their newsletter (*NeWS*) were distributed which showed what the chemical societies of Canada, Japan and Australia were planning to do. Further information about the plans of the International Chemistry Celebration (IChC) in 1999 may be found on their web site:

http://www.acs.org/memgen/meetings/ichc/ichc.htm

Chemistry teaching and the Internet

Becky Allen

The Royal Society of Chemistry (RSC) is the National Chemical Society of the United Kingdom. The RSC webmaster Becky Allen looks at some key chemistry teaching web sites and asks a group of chemistry teachers from Cambridge (UK) what they think of the Internet as a resource.

Chemistry teachers in Cambridge have recently run workshops examining the potential promise and pitfalls of using the Internet, and more specifically the World Wide Web (WWW), in schools. The RSC's new media department, responsible for the launch of the RSC's own server a year ago, has developed a web page of chemistry teaching resources to provide a focus for these and future workshops, and to stimulate debate on the value of web technology to chemistry teachers at all levels.

The school net

Dozens of schools are connecting to the Internet each week and acceptance of this new technology is finally filtering down to even the most technophobic teachers, according to Dr John Baruch of Bradford University's industrial technology department. He predicts that 'next year the net will take off in schools', and is himself involved in researching methods of using the Internet in classrooms. Phase one of his work involves developing multi-user dungeons (MUDs) to create virtual classrooms which allow students from different schools, within the same city, to talk each other. He is also writing a handbook for teachers and IT staff on how to get the most out of using the Internet. Schools need long-term plans to exploit Internet teaching resources he believes, including networking their PCs, investing in ISDN lines rather than modems, and establishing appropriate hardware and software. IBM-compatible PCs running Windows 3 or 3.1, he says, are the way forward.

Although many teachers think cost is a major hurdle, Dr Mike Carrington, from Hills Road Sixth Form College, Cambridge, UK, is not so sure. 'Most schools should have suitable hardware and the additional costs involved in buying a good modem and getting on-line through a provider are within the budget of many households, so surely should be relatively easy to finance for even small schools', he says. He also thinks that many teachers lack experience of using the Internet, its associated software (browsers and

authoring tools), and the time to find useful web sites on a range of topics to include in work schemes. Although he has used the web for extension work, getting students to do library projects to widen their research to CD-ROM and the Internet, 'without time for teachers to investigate what is available, and with a large proportion of kids being first time users, the pay-back on early use by students has been very patchy'.

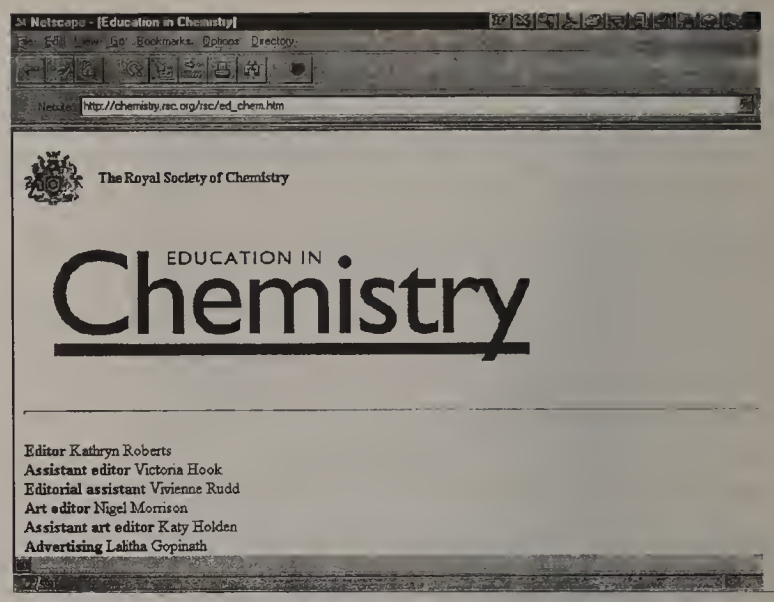
Karen Marshall, at Impington Village College, near Cambridge, believes that the benefits outweigh the costs. 'It is extremely short-sighted of schools as well as an economy drive to feel that it [the web] is not one of the most important developments of the present day'. She has used the web to view real-time telescope pictures, access planetary data from the NASA Home Page, research information about nuclear power and access WebElements for Year 9 extension work. She believes the web is suited to all ages and that although it may be much more fun doing chemical reactions than using the Internet, the links it provides to other parts of chemistry make it a very useful tool.

Adam Drury of the Chemistry Teaching Consortium/ Computers in Teaching Initiative at the University of Liverpool (UK) also thinks that the web is maturing into a useful resource for teaching: he believes that initial drawbacks are being overcome, but points out that bandwidth remains a problem. 'The web is still slow, particularly if you want to access material...in the US in the European afternoon'.

The web is, of course, only one part of the Internet, and schools could exploit other areas such as email and discussion lists more fully. More and more companies have web sites giving email addresses, to which students can easily and quickly send queries. The trend towards increased emphasis on industrial and environmental aspects of chemistry at A-level (exams taken by high school students at age 18) should give more scope for web use.

Among the growing band of chemistry teachers using email discussion lists is Alastair Gittner of Hinchinbrooke School in Huntingdon (UK). 'By far the most useful [part of the Internet] to me is my subscription to a chemistry listserv, which has produced lots of helpful ideas and comments on all aspects of chemistry teaching despite its US bias'. Gittner has groups of students involved in a world-wide project using email to pool data on water usage, rainfall and purification with other schools as far afield as North America, Australia and the Bahamas. Although he wants students to concentrate on the science first, he feels many are not computer literate enough to be given free rein to surf themselves. 'We are trying to teach the use of the Internet as just one more resource', he says.

Gittner is also involved with the Association for Science Education's Science across Europe scheme,



***Education in Chemistry* on the web: http://chemistry.rsc.org/rsc/ed_chem.htm**

which is curriculum-linked and uses the Internet. The work, centred around water supply, pollution and purification across Europe, involves students using both CD-ROM and the Internet to gather data. 'I have also built into the project the basic aim that all pupils should learn how to send and receive email at the end of this unit'. Although he believes that being able to communicate with other people across the world will be very rewarding for pupils, he is concerned that pupils may have access to too much information but lack the skills to sort it out. 'We run the risk of kids knowing nothing but just knowing where to go and look it up', he says, 'and I have not seen any structured activities to lead the pupils to sensible use of the web'.

Awareness then, needs to be raised among both students and teachers. The following is a brief introduction to some of the sites chemistry teachers are using as resources for classroom activities, sources of information on the technology itself, and as a means of exchanging ideas and sharing experiences. Their Internet addresses, or URLs, are given in the box, and can be directly accessed from the RSC web server at http://chemistry.rsc.org/rsc/teachers.htm

Classroom resources

A wide variety of chemistry teaching resources already exists on the web, some sites simply bringing the work of existing organizations to a wider audience, but others owing their existence to the possibilities the web has opened up. Web sites provided by existing organizations with a proven track record also make it easier to rely on the source and accuracy of information on the Internet, a major concern for most Internet users, including teachers. Existing organizations such as the Network for Chemistry Teaching and the Association for Science Education fall into this first category. Although these sites can be primarily promotional in content, they nevertheless provide valuable information on

the work of organizations that some teachers may not be directly involved with but could benefit from monitoring with the ease that a web site allows.

Other groups that have a much more synergistic relationship with the web include the National Council for Educational Technology (NCET), Schools OnLine, eLABorate, Chemical Education Hypermedia and the Computers in Teaching Initiative. While these have a wider educational remit than chemistry alone, such web sites are showcases for some of the most innovative science teaching work on the web. NCET acts as an agent for several UK government departments in managing the Education Department's Superhighway's Initiative, involving GBP 9.4 million in 23 projects, including Science across Europe. The NCET web site details this and other projects, contains a list of educational URLs, teachers' and students' guides on chemical topics (rates of reaction and catalysts), and the IT for Teachers project.

Schools OnLine is now at the end of its one year pilot, but its server will remain active until September. Funded to the tune of GBP 1 million by the Department for Trade and Industry and commercial partners, Schools OnLine brought together Higher Education research, schools and companies seeking 'to offer students a positive, creative role, not just looking at "interesting stuff" on the web, but participating in projects, collaborating and creating material...pushing forward the concept of what can be done with web pages'.

The original proposal of eLABorate, a project funded by the UK Higher Education funding bodies as part of phase two of their Teaching and Learning Technology Programme and distributed over UK universities at York, Leeds, Surrey and Oxford, was to design and prepare computer simulations of laboratory experiments, enabling chemistry and biochemistry students to develop skills in planning experiments, optimizing procedures and interpreting data.

Chemistry teachers Kurt Irgum in Sweden and Patrick Gormley in the US are building impressive web sites with pointers to myriad science teaching resources. Patrick Gormley's site, Science Teaching Resources, has been set up for science teachers to share ideas. Gormley aims to provide labs, demonstrations and other information for teachers to access.

Among the email discussion lists is Chem-education, where chemistry teachers are currently busy sharing thoughts and research on standards of maths among chemistry undergraduates. Other innovative features are the development of tutorial mark-up language by Bristol University's Dr Paul May, which allows students to test their own chemistry knowledge via interactive web pages, and WebElements from Sheffield University's Dr Mark Winter. This electronic Periodic Table represents a highly attractive way to research an element's chemical, physical, nuclear, electronic, biological, geographical and crystallographic data. University chemistry departments are also experimenting with web archives of notes for students; hypermedia tutorials;

Other Internet resources

The Royal Society of Chemistry	http://chemistry.rsc.org/rsc/
Bradford University Robotic Telescope	http://www.telescope.org:80/rti/
CTC/CTI	http://www.liv.ac.uk/ctichem.html
NCET	http://ncet.csv.warwick.ac.uk
Tutorial Markup Language	http://www.ets.bris.ac.uk/ets/resource/tutorial/tutorial.htm
Principles of Protein Structure	http://www.cryst.bbk.ac.uk/pps2/
Science Teachers Resources	http://www.lapeer.lib.mi.us/chem/eastscires.html
Chemistry Teaching Resources	http://www.anachem.umu.se/eks/pointers.htm
Network for Chemistry Teaching	http://euler.ntu.ac.uk/rwa/homepage.html
chem-education list, to join send text 'join <chem-education> <firstname> <lastname>' to	mailbase@mailbase.ac.uk
eLABorate	http://www.york.ac.uk/depts/chem/staff/elaborate
ASE	http://www.rmplc.co.uk/orgs/asehq/index.html
Chemical Education Hypermedia	http://www.chem.vt.edu/chem-ed/vt-chemed.html
Schools OnLine	http://sol.ultralab.anglia.ac.uk/pages/schools_online/
Science OnLine	http://www.shu.ac.uk/schools/sci/sol/contents.htm
National Institute for Science Education	http://www.wcer.wisc.edu/nise/
WebElements	http://www.shef.ac.uk:80/~chem/webelements/
ChemEd	http://www-hpcc.astro.washington.edu/scied/chemistry.html

and the Principles of Protein Structure course—a pioneering experiment in the virtual delivery of knowledge solely using the web. The US National Institute for Science Education web site is currently debating whether the web has a role in improving science (and especially chemistry) education in schools.

Acknowledgements

Thanks to all the teachers who contributed to this feature, mostly in the form of email interviews; if others have experiences to share, or feedback on any of the sites mentioned, or overlooked, please contact Becky Allen (editor, internet services), the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge CB4 4WF, UK (email: allenb@rsc.org).

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White Book on Chlorine

The September, 1996, issue of *Pure & Applied Chemistry* is given over entirely to a consideration of the use of chlorine in our society. As chemists, we are aware that chlorine together with products containing, and made from chlorine containing molecules are essential in our society. Such materials have enhanced our lives and improved our living standards, however, there has been much concern within the wider community about the widespread use of chlorine and chlorine containing materials.

It is hoped that a detailed public understanding of the versatility and essentialness of chlorine will encourage debate about its future, and try to ensure that decisions about the continued use of chlorine containing materials are made on the basis of sound judgement and proven science, and not on alarmist reports.

This special issue of *Pure & Applied Chemistry* is intended to stand alone as one of the well-known IUPAC colour books—the White Book. This White Book contains articles by well known experts on the occurrence of chlorine and chlorine products in nature, the production and applications of chlorine, and on environmental and health issues related to chlorine and chlorine containing materials. There is a conclusion, written by the President of IUPAC, Prof. Albert E. Fischli, which puts the current alarm about chlorine in the non-chemical community in perspective.

It is hoped that this volume, prepared by experts from around the world, who evaluate critically various aspects of this subject will be of interest not only to academic institutions, industry, governmental agencies and environmental organizations, but also to the general public.

The White Book is the first publication by IUPAC of this type. Similar analyses are envisaged of the chemical aspects of other globally important issues, in which IUPAC can play a role, standing firmly on a scientific foundation independent from governments and industry, by calling on its world-wide network of experts from various fields of chemistry.

Chlorine—an introduction

George Porter (Chairman, Centre for Photomolecular Sciences, Imperial College of Science Technology and Medecine, London SW7 2AY, UK)

Chlorine, in the form of its salts, has been known since the earliest days of recorded history, although its recognition as an element did not occur until the beginning of the 19th century when its very high reactivity as an oxidant was found remarkable after it was shown not to contain any oxygen. Its absorption by sunlight made it a key substance in the early development of photochemistry. One example of this, with both pure and applied

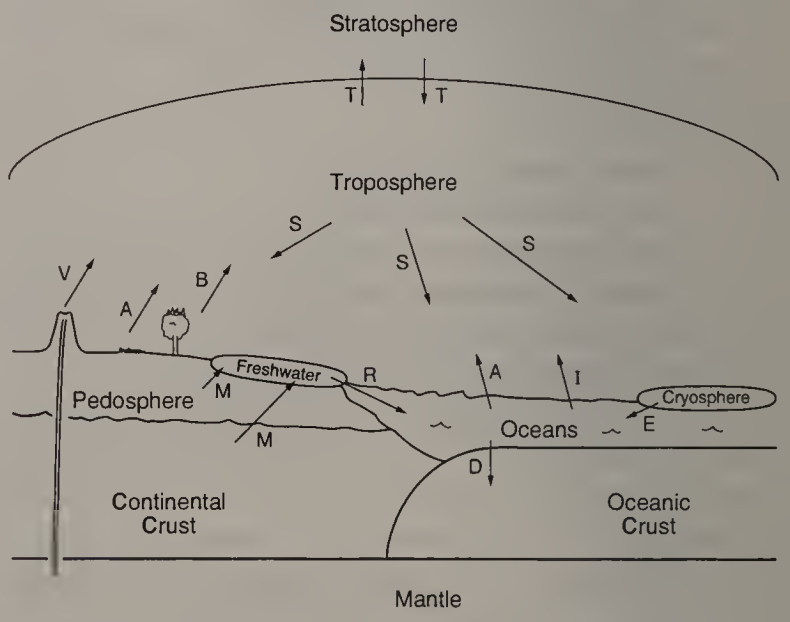

Fig. 1 The planetary chlorine reservoirs. The natural processes transferring chlorine among the reservoirs are: A, algae and fungi; B, biomass burning; D, diagenesis, E, elution; I, sea spray injection; M, mineral dissolution; R, runoff; S, surface deposition; T, turbulent mixing, and V, volcanism. See *The Budget and Cycle of Earth's Natural Chlorine* for full details.

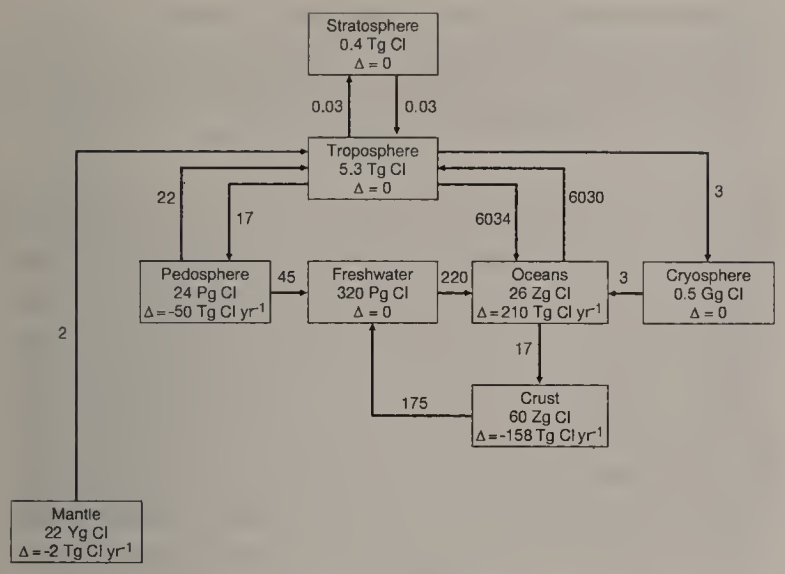

Fig. 2 The chlorine budget and cycle for the five planetary reservoirs. The fluxes and reservoir content changes are in units of Tg/year. The processes responsible for the transfers are given in the caption to Fig. 1. See *The Budget and Cycle of Earth's Natural Chlorine* for full details.

aspects, is described in more detail. The free radical chloric oxide played an important role in the development of the technique of flash photolysis and 25 years later these researches were of essential importance in showing how chlorine and its oxides were involved in the destruction of the ozone layer by the chlorofluorocarbons.

The budget and cycle of Earth's natural chlorine

T.E. Graedel[1] and W.C. Keene[2] ([1]Bell Laboratories, Lucent Technologies, Murray Hill, NJ 07974 USA; [2]University of Virginia, Charlottesville, VA 22903 USA)

Earth's chlorine, retained when the planet was formed from the Solar nebula, is contained largely in three reservoirs: the mantle (99.6%), the crust (0.3%), and the oceans (0.1%). Only oceanic chlorine is readily mobile, cycling among the lower and middle atmosphere, the pedosphere, freshwaters, and the cryosphere. Inter-reservoir chlorine fluxes are estimated for all transitions of interest; by far the most important on a mass basis is the injection of seasalt from the oceans to the atmosphere, and its return to the planetary surface by wet and dry deposition.

The diversity of natural organochlorines in living organisms

G.W. Gribble (Department of Chemistry, Dartmouth College, Hanover, New Hampshire 03755, USA)

Of the more than 2600 known naturally occurring organohalogen compounds, more than 1500 contain chlorine. These organochlorines, which range in structural intricacy from the ubiquitous fungal and plant metabolite chloromethane to the complex life-saving antibiotic vancomycin, are produced by marine and terrestrial plants, bacteria, fungi, lichens, insects, marine animals (sponges, sea hares, nudibranchs, gorgonians, tunicates), some higher animals, and a few mammals. New examples are continually being discovered and the total number of natural organohalogens may surpass 3000 by the turn of the century.

The chlorine industry

Jacqueline Fauvarque (Ecole Supérieure de Chimie Organique et Minérale (ESCOM), Centre Polytechnique Saint Louis, 13 boulevard de l'Hautil, 95092 Cergy-Pontoise, France)

Numerous products, such as polymers, chemicals or pharmaceuticals and ultra-pure metals, which often do not actually contain chlorine, are produced using either chlorine or its derivatives. They are essential in all industrial sectors and in our daily lives. New chlorine production units have adopted the membrane electrolytic process, but the century-old diaphragm and mercury processes retain their high-performance characteristics when appropriately modernised and improved.

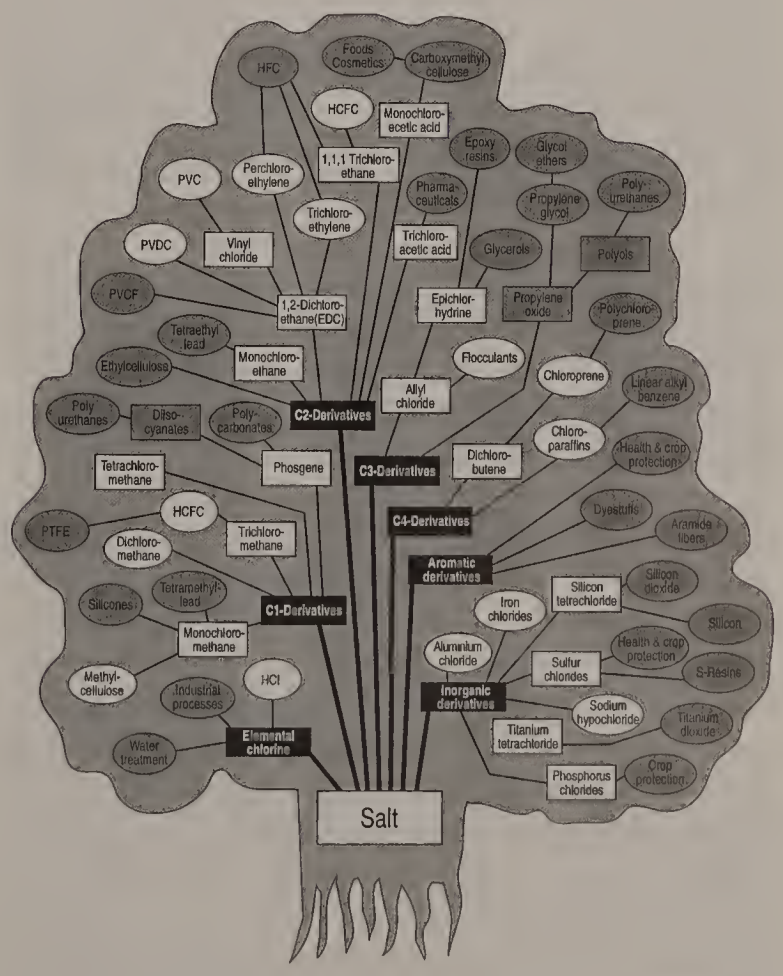

Fig. 3 The chlorine tree—showing the origin of manufactured chlorine products, see *The Chlorine Industry* for full details.

Chlorine in the bleaching of pulp and paper

K.R. Solomon (Centre for Toxicology, University of Guelph, Guelph ON, N1G 2W1, Canada)

The pulp and paper industry in Canada contributes significant effluent discharges to surface and marine waters. Chlorine and chlorine compounds are used in the bleaching of pulp. A large number of organochlorine chemicals of widely differing properties are, or have been, produced from this bleaching. These range from the highly hydrophobic, persistent and bioaccumulative toxic substances, such as 2,3,7,8-TCDD, to the higher molecular weight, non-hydrophobic material usually characterized by absorbable organic halogen. Chlorine dioxide and chlorine react with lignin by different chemical processes and produce different organochlorine products. Use of molecular chlorine as a bleaching agent results in the formation and release of chlorinated organic compounds, sometimes at concentrations that present an unacceptable risk to the receiving environment and the food chain. Alternatives to the use of molecular chlorine, such as chlorine dioxide, result in reductions in the quantities of organochlorines produced, and the degree of chlorine substitution in the organochlorines formed. This, in turn, leads to reduced persistence, reduced potential for bioaccumulation and food chain transfer, reduced toxicity and reductions in adverse ecological effects. However, sufficient evidence exists from responses observed at non-bleached mills to show that other (probably non-halogenated) compounds are released or formed during the production of pulp and cause responses such as induction of MFOs, changes in hormone levels, and reproductive effects.

Chlorine in water disinfection

H. Galal-Gorchev (International Programme on Chemical Safety, World Health Organization, Geneva, Switzerland)

Disinfection of drinking-water is one of the main achievements of our time in the protection of public health. The use of chlorine for the destruction of microbiological pathogens is essential to protect the public from outbreaks of waterborne disease. Chlorine, as well as other disinfectants, produces a variety of chemical by-products. The risk from the presence of microbial pathogens in drinking-water is estimated to be several orders of magnitude greater than the risk from chlorination by-products. Any efforts to control these by-products must not compromise the microbiological quality of drinking-water.

Environmental and health issues

J. Miyamoto (President, IUPAC Division of Chemistry and the Environment)

The environmental behaviour of a chemical is governed by its intrinsic physicochemical properties, including their metabolic activities, as well as by characteristic features of the environmental compartments. This inextricable network of interactions contribute to degradation and mineralization of organic compounds. Under the circumstances that the chemical is lipophilic and/or resistant against chemical and biological degradation, it tends to be transported to other environmental compartments and/or subject to bioaccumulation. The adverse effects of chemicals on humans and organisms in the environment are assessed by a variety of toxicological studies to establish ADI (acceptable daily intake in man) or PNEC (predicted no observed effect level in organisms), in comparison with the calculated exposure levels based on the environmental behaviour of chemicals.

The role of chlorine in stratospheric chemistry

M.J. Molina (Departments of Earth, Atmospheric and Planetary Sciences and Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139, USA)

The chlorofluorocarbons (CFCs) are industrial chemicals used as solvents, refrigerants, plastic foam blow-

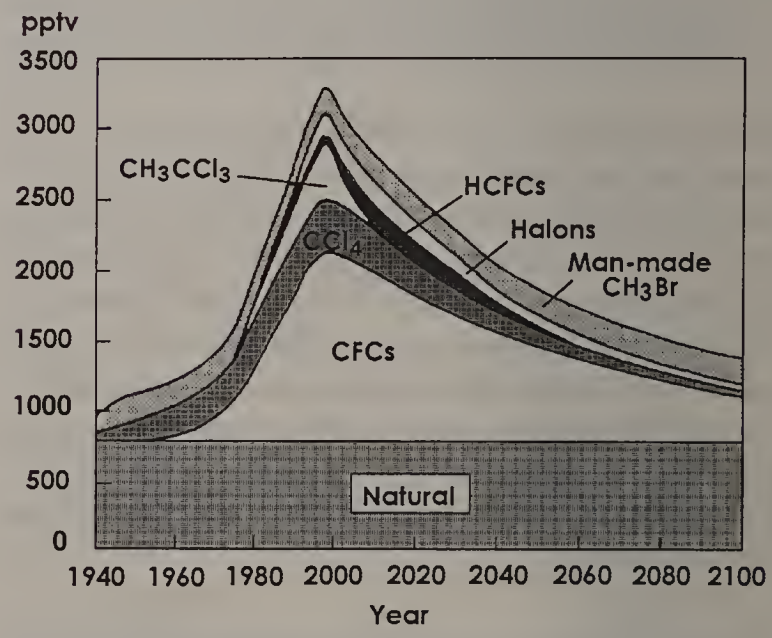

Fig. 4 Stratospheric reactive halogen loading (taken from Alternative Fluorocarbons Environmental Acceptability Study. *AFEAS Brochure* (1995). Alternative Fluorocarbons Environmental Acceptability Study. *Production, sales and atmospheric release of fluorocarbons through 1994.* AFEAS, The West Tower—Suite 400, 1333 H Street NW, Washington DC 20005, USA (1995)), for full details see *The Atmospheric Fate and Impact of Hydrochlorofluorocarbons and Chlorinated Solvents.*

ing agents, etc. These compounds are eventually released to the environment; they slowly drift into the stratosphere, where they decompose, initiating a catalytic process involving chlorine free radicals and leading to ozone destruction. The stratospheric ozone layer is important for the earth's energy budget, and it shields the surface of the earth from ultraviolet radiation from the sun. Very significant depletion of the ozone layer has been observed in the spring months over Antarctica during the last 10–15 years. Laboratory experiments, model calculations and field measurements, which include several aircraft expeditions, have yielded a wealth of information which clearly points to the CFCs as the main cause of this depletion.

The atmospheric fate and impact of hydrochlorofluorocarbons and chlorinated solvents

Howard Sidebottom[1] and James Franklin[2] ([1]Department of Chemistry, University College Dublin, Belfield, Dublin 4, Ireland; [2]Alternative Fluorocarbon Environmental Acceptability Study (AFEAS), The West Tower—Suite 400, 1333 H Street NW, Washington DC, USA.

A very considerable body of data pertaining to the atmospheric behaviour of hydrochlorofluorocarbons (HCFCs) and chlorinated solvents is now available and leads to the following conclusions: (a) these compounds, with the exception of 1,1,1-trichloroethane, make a small or insignificant contribution to stratospheric ozone depletion, global warming, 'photochemical smog', 'acid rain', or chloride and fluoride levels in precipitation; (b) it seems highly unlikely that the chlorinated solvents degrade in the atmosphere to give chloroacetic acids as major products, as has often been claimed in the literature.

Persistent, ecotoxic and bioaccumulative compounds and their possible environmental effects

K. Ballschmiter (University of Ulm, Department of Analytical and Environmental Chemistry, Albert-Einstein-Allee 11 D-89069 Ulm, Germany).

The relationship between physicochemical properties, environmental distribution and effects of organochlorine compounds as a major class of persistent organic pollutants (POPs) are discussed. The environmental fate of a compound includes its transport and dispersion in the environment as well as its accumulation and transformation in defined environmental compartments. Accumulation and transformation as the result of environmental distribution may have long-term consequences; this is indicated by the ultimate accumulation and long-term bioactivity of several widely spread organochlorines, and is clearly evident in the decomposition of chlorofluorocarbons in the stratosphere.

Depending on the order of trophic levels biomagnifiaction factors of 10 000 up to 100 000 are encountered for persistent semivolatile organochlorines such as 4,4′-DDE, PCB congeners or some Toxaphene constituents. Mammals show intraspecies pollutant transfer during the lactation period. While the mother animal is partly depleting its body burden, the calve accumulates in a critical period of its life via the milk a concentrated input of persistent organochlorines. A similar depletion phenomenon is also found for fish and crustacean which enrich in the eggs a substantial part of the accumulated body burden of the female.

The air skimming of semivolatiles by plant surfaces leads to surprisingly high levels of pollutants in the upper soil layers of forests that otherwise would be considered pristine in terms of human activities.

Sources and environmental concentrations of dioxins and related compounds

Christoffer Rappe (Institute of Environmental Chemistry, Umeå University, S-901 87 Umeå, Sweden)

Polychlorinated dioxins and dibenzofurans are two series of tricyclic aromatic compounds, which have been the focus of the interest in the last decades; in all there exist more than 200 congeners. They are formed in numerous ways, primarily in incineration processes and in industrial processes. It has also been found that they are formed by natural processes. They are ubiquitous and have been quantified in abiotic samples such as soil, sediments and air as well as in living organisms, primarily aquatic organisms. A dramatic decrease in most environmental concentrations including biological and human samples of PCDDs and PCDFs has been identified. There is a discrepancy between sources and environmental reservoirs which cannot be fully explained.

Toxicology of environmentally persistent chlorinated organic compounds

Annika Hanberg (Institute of Environmental Medicine, Karolinska Institute, Box 210, S-171 77 Stockholm, Sweden).

The chlorinated organic compounds comprise a large group of compounds with a complex diversity of biologic effects and mechanisms of action. Based on the

persistence and high toxicity of dioxins, PCBs, and DDT, this chapter focuses primarily on the toxicology of these organochlorine compounds. Not even these groups of compounds can be regarded as homogenous since the individual congeners show diverse environmental fates and toxicities. In this chapter, we will consider primarily the critical effects suspected to occur at human exposure at background levels, i.e. cancer, and effects on reproduction, neurobehaviour and the immune system. In recent years, interactions between these compounds and hormonal systems have received increasing attention. They have also been shown to be particularly toxic to the developing embryo, foetus and infant. In order to conduct accurate risk assessment, there is a need for further mechanistical data, and additional epidemiological studies, especially with regard to effects on reproductive, neurobehavioural and immune systems. The data presently available suggest that such effects already occur in the human population and thus, in order to reduce the exposure to these compounds, further release into the environment should be prevented.

Organochlorine waste management

Roger Papp (Chairman of the Scientific and Technical Committee of CNEEIC (College National d'Experts Environnement de l'Industrie Chimique France, and Professor of Chemical Engineering, Ecole Centrale de Paris, France).

Sound environmental management includes the proper management of waste. This chapter reviews the basic rules of good management practice illustrated by some examples from chlorine derivatives production and gives the main considerations governing the Best Available Techniques for organochlorine waste thermal treatment. A review of the main degradation pathways of organochlorines—dispersal, distribution, degradation pathways, and environmental half-lives—demonstrates a very large range of characteristics, justifying the need for a separate study for each substance. Finally, the paper examines the latest developments in organochlorine contaminated site remediation technology.

PVC recycling management

G. Menges (Institut für Kuntstoffverarbeitung in Industrie and Handwerk an der Rheinisch-Westfälischen Technischen Hochschule, Aachen, Germany)

PVC is the second most important polymer world-wide. Thanks to its excellent cost/performance ratio and outstanding chemical and environmental resistance, it is today mainly used for long-life applications. In some countries, for example, France, PVC is used in large volume for the manufacture of bottles. Pure PVC scrap can be recycled without any problems. Although many applications for such products of recycled PVC have been developed, and pilot plants for recycling exist, only small volumes have been recycled up to now. Only bottles made from PVC for the large drinking water market in France are already collected separately, recycled in large quantities, and transformed into such articles as water pipes. Specialist organizations deal with this business. In such cases, for example, kitchen waste, where PVC is part of mixed plastics waste for example, sorting and separation of the PVC is necessary.

Conclusions

Albert E. Fischli (IUPAC President)

A crusade is ongoing against element 17 in the periodic table, i.e. chlorine, one of the most abundant on earth. It is blamed, amongst other things, to be responsible for the depletion of the ozone layer, bioaccumulation of chlorinated compounds such as DDT or PCB's in animals and for the formation of dioxins in urban waste incineration.

Due to socio-economic implications the issue has gone too early beyond the borders of the scientific community, before facts have been proven and evaluated. As a result, it has been treated in inappropriate and emotional ways even affecting scientific ethics in some cases.

Therefore, the International Union of Pure and Applied Chemistry (IUPAC), conscious of its responsibilities in this area, has decided to publish this White Book with the collaboration of outstanding worldwide renowned scientific specialists from North-America, Europe and Japan in order to inform the public and the decision makers as well as the scientific community in an objective, open and unbiased way on the up-to-date scientific knowledge.

In doing so IUPAC is following its philosophy to make independent judgments on important issues that are touchy or sensitive to the general public, governments and industry. IUPAC is not acting as a judge, but would like to critically evaluate the various factors for and against a particular issue.

The occurrence of chlorine in nature and also in living organisms, either as inorganic compounds or as numerous and very diversified natural 'organochlorines' doesn't make any doubt any more (T. Graedel and W.C. Keene, G.W. Gribble).

The availability of the raw material, salt, the development of convenient production technologies and the chemical properties of chlorine have generated a blooming tree of applications in such different fields

as the pulp and paper industry (K. Solomon), the disinfection of water (H. Galal-Gorchev) but mainly in organic synthesis leading to a host of useful products, for example, polymers, pharmaceuticals, pesticides, dyes and pigments (J. Fauvarque).

It is quite clear that chemists have not always been aware beforehand of all the possible consequences of having manufactured new molecules, be they chlorinated or not. Chemicals emitted voluntarily or inadvertently in the environment are distributed there according to a complex set of physico-chemical properties (J. Miyamoto, K. Ballschmiter).

Volatile compounds such as aliphatic chlorinated and chlorofluorinated hydrocarbons find their way to the 'atmospheric compartments'. Long-lived members of this family are even able to reach the stratosphere where they have been shown to produce detrimental effects to the global environment (M. Molina).

The substitution of these so-called CFCs by new shorter-lived molecules has probably been the best example of a sound scientific approach to solving environmental problems. A host of scientific studies has shown that short-lived chlorinated aliphatic compounds make only minor or even insignificant contributions to environmental problems such as stratospheric ozone depletion, global warming, 'photochemical smog', 'acid rain' or chloride levels in precipitations (J.A. Franklin and H.W. Sidebottom).

Are organochlorines harmless or harmful? The question seems as irrelevant as asking if natural compounds are harmless and anthropogenic ones toxic.

Ecotoxicity (K. Ballschmiter) and toxicity (A. Hanberg) as any other 'chemical' property of any compound depends on the structure of its molecule; chlorinated or otherwise halogenated compounds do not escape this rule. Therefore, an undifferentiated ban of whole classes of chemical compounds has to be qualified as unscientific.

Even in apparently 'homogeneous' families such as the dioxins, toxicity varies considerably with the position and the number of substituents (Ch. Rappe). There is thus no scientific foundation to the amalgamation of all chlorinated compounds as a group showing special toxic and ecotoxic properties, no more than one should consider organo-oxygens or organo-nitrogens as a whole as harmful because highly toxic warfare agents as sarin or tabun contain these atoms in their molecules.

This obviously doesn't mean that organo-chlorine waste, as any sort of waste, has not to be managed. The problem has been tackled and technical solutions have been developed to reduce byproducts formation by improving the production processes, to destroy and/or vaporize the remaining production wastes (R. Papp). This has now to be generalized in the most economic and environmentally friendly ways. In some cases, post-use recycling is being developed and starts to be generalized as for the recycling of PVC for which 'second life' applications have been found (G. Menges).

In conclusion, I would like to add a few words formulated by the Nobel laureate Prof. Lord George Porter earlier on. 'There is no way that humans can foresee all the consequences of their actions,...The only sure foundation for security in this technological world is to have a science base which is continually asking whatever questions seem interesting and is always there to advise and to act when the need emerges.'

It is the responsibility of the scientific community to develop this science base, of the media to help them to inform the public in an understandable and unbiased way, of the public authority to take the relevant decisions on the bases of sound science and not on emotional reactions and of industry to act responsibly, endorsing product stewardship and responsible care. This is true for chlorine and its chemistry as well as it is for all human activities.

There are two organizations established to promote and protect the use of chlorine and chlorine containing materials by industry. The Chlorine Chemistry Council was established in 1993 to participate in the public policy debate surrounding chlorine chemistry. In this role, the Chlorine Chemistry Council develops and implements proactive programs promoting the benefits of chlorine chemistry, and the practice and understanding of responsible management, or stewardship, for chlorine chemistry and chlorine-based products. The Council also identifies and responds to health and environmental issues that involve chlorine chemistry and chlorine-based products.

Specific activities of the Chlorine Chemistry Council are aimed at:

Science: Facilitating comparative risk and risk benefit analyses through the collection, development, and use of scientific data on health and environmental issues surrounding chlorine chemistry.

Stewardship: Fostering protection of human health and the environment in the production, distribution, use, and disposal of the products of chlorine chemistry.

Outreach: Heightening public awareness of chlorine chemistry and its many societal benefits through the development and implementation of communications programmes.

The Council membership includes all leading US chlorine

producers. The Chlorine Chemistry Council, a business council of the Chemical Manufacturers Association, is comprised of manufacturers and users of chlorine and chlorine-based products, and other organizations with an interest in chlorine chemistry. With a long-term commitment to balanced classroom discussions of science and the environment, the Chlorine Chemistry Council has become associated with several nationally recognized education organizations to develop quality education programs and materials. The Chlorine Chemistry Council is located in Arlington, VA, USA

For further information, see the Internet Home Page of the Chlorine Chemistry Council (http://c3.org).

The Chlorophiles are an independent non-profit organization of workers in the chlorine and PVC industry who want to react to the allegations against their endeavours. They point out that they work responsibly and with care to manufacture products for the well being of society. They note that mankind should not be excluded from the benefits of chlorine and chlorine products on the basis of prejudice and false or erroneous information.

For further information, see the Internet Home Page of the Chlorophiles: http://www.ping.be/~ping5859/Eng/chlorophiles.html.

Additional information about the background to the current debate on the environmental impact of chlorine and chlorine containing compounds on the environment may be found at:

http://www.cis.ohio-state.edu/hypertext/faq/usenet/ozone-depletion/stratcl/faq-doc-5.html

High temperature copper oxide superconductors

Ever since its discovery by Kammerlingh Onnes in 1911, superconductivity has fascinated scientists. The superconducting state is one which offers no resistance to the passage of an electrical current and repels an applied magnetic field. The first superconductor was Hg cooled below 4.2 K. Indeed, it is a phenomenon which required the technological advance of the liquefaction of helium for its discovery. By March 1913, Kammerlingh Onnes was able to present his first results and refer to 'the superconductivity of mercury', thereby naming the effect. Since this date, just about every new material has been investigated for its superconducting properties. Figure 1 shows how the temperature of the transition from the nonsuperconducting state to the superconducting state crept slowly upwards until the discovery of the ceramic cuprate materials. Thereafter the evolution of the superconducting transition temperature has been spectacular, but it has slowed down of late.

The discovery of superconductivity has—apart from a limited number of technological applications due to the necessity of maintaining extremely low temperatures for conventional superconductors—led to the facinating phenomenon of macroscopic quantization. That is, the whole superconducting sample being described by a single wavefunction—the manifestation of the laws of quantum mechanics not on atomic dimensions, but on the scale of macroscopic laboratory samples.

Superconductivity arises when electrons, which normally repel each other electrostatically, form pairs—Cooper pairs—which then condense into a single macroscopic quantum state. Single electrons are fermions which obey the Pauli exclusion principle: only one of each spin may occupy the same energy level—as in a conventional covalent chemical bond. The coupled electrons, Cooper pairs, are bosons of which any number may occupy the same quantum level. The Cooper pair bosons therefore condense into a single macroscopic quantum state with a coherent phase. However, this coherence of the electron pairs is strongly coupled to the nuclear material present in the lattice and it is this strong coupling or perturbation which has made a theoretical understanding of the new high temperature cuprate superconductors so elusive.

In order to bind, electrons have first to overcome the electrostatic repulsion between them. This requires the presence of a strong attractive interaction which overcomes the Coulomb repulsion between like-charged particles. The Bardeen–Cooper–Schrieffer (BCS) theory of superconductivity successfully accounts for the attractive interaction present in classical low temperature superconductors—those known before the hiatus of the cuprate superconductors. In the BCS theory, the attractive interaction between the electrons arises from their respective interaction with the vibrations of the solid lattice, the phonons. Thus, each electron interacts with the lattice vibrations and the sum of these attractive interactions exceeds the repulsive Coulombic interaction between the electrons. There is therefore a net attractive interaction between a pair of electrons mediated by the lattice phonons. The BCS theory works well at low temperatures, and shows how, as the temperature rises, the phonon motion becomes nonquantized and chaotic and the net attractive inter-

action with the electrons vanishes and the sample losses its superconductivity.

To try and understand how one might envisage overcoming the strong electrostatic repulsion between like-charged species and obtain a net attractive interaction which will lead to a pairing, one may think of a chemical analogy with two like-charged ions in a polarizable medium. For example, two anions in an aqueous solution. There is the classic Coulombic repulsion between the similarly charged ions and they will not, under these conditions, approach one another closely. However, the polarizable medium may be polarized by ion 1 so that it becomes attractive to a nearby ion 2 of the same polarity, but repulsive to an ion of opposite polarity. There is a net induction energy arising from the electric fields E_1 and E_2 of the two ions, proportional to $(E_1 + E_2)^2$ and the cross term will cause an apparent attraction between ions of like polarity. Considerations of dimensions show that the presence of sufficiently polarizable material between like-charged particles can give rise to an attractive force greater than the simple ion–ion Coulombic repulsion.

There are various theories for the new high temperature superconductors. However, they disagree on the origin of the attractive interaction between the electron pairs. At issue is the internal state of the electron pair. Do the pairs have an angular momentum value of 0, in which case they are said to occupy an *s*-wave state

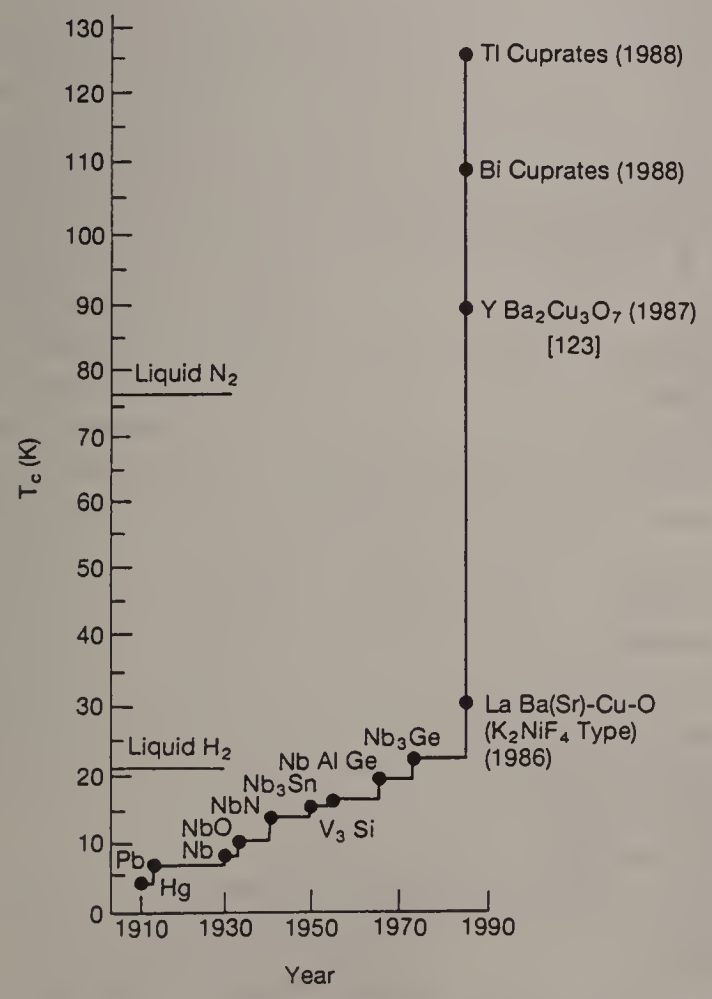

Fig. 1 Evolution of superconducting transition temperatures (taken from C.N.R. Rao, *Chemistry of Advanced Materials*, Blackwell Scientific Publications, 1993).

Table 1 Superconducting transition temperatures

Material	T_c (K)
Hg	4.2
Nb	9.5
$C_{60}K_x$	18
$La_{1.8}Sr_{0.2}CuO_4$	35
$TlSrLaCuO_5$	40
$YBa_2Cu_3O_7$	92
$Bi_2(CaSr)_3Cu_2O_8$	90
$Bi_2(CaSr)_4Cu_3O_{10}$	110
$Tl_2Ca_2Ba_2Cu_3O_{10}$	125
$(Ba,Sr)CuO_2$	90

(think of the analogy with an *s*-orbital in an atom), or are the electron pairs formed from states with an angular momentum of 2, in which case they are said to be in a *d*-wave state (again think of the analogy with the *d*-orbits in atoms). Current evidence is in favour of the *d*-wave hypothesis; however, the debate is by no means closed.

The first mention of copper oxide superconductors to the unsuspecting world was in 1986 with the discovery of superconductivity in the La–Ba–Cu–O system (structure 0201 in the following compilation) by J. G. Bednorz & K. A. Müller (*Z. Phys. B.* 1986, **64**, 189). Since this first report, hundreds, perhaps even thousands, of materials have been synthesized and examined for evidence of superconductivity. Indeed, the search for materials with ever higher transition temperatures to the superconducting state has engendered a whole new interest in high temperature solid state inorganic chemistry. Table 1 gives an idea of the change in the transition temperature from nonsuperconducting state to the superconducting state seen in these new materials and in some classic superconductors.

Almost without exception, the crystal structures of these cuprates are characterized by superconducting CuO_2 sheets that are separated by nonsuperconducting planes. These structures possess features closely related to the classic perovskite ($CaTiO_3$) structure, such as vertical-sharing metal-centered octahedra, square pyramids, square chains and chains. Since all these new materials are composed of similar building blocks it is useful to classify these cuprates in terms of their common structural features. Needless to say, the structurally unique copper oxide superconductors do not all have the same structure; there are important structural subtleties such as the tilting of the copper oxide octahedra and the buckling of the metal oxide spacing layers which determine the actual temperature at which the material becomes superconducting.

As these materials are now investigated in many laboratories, simple classifications based on the structural units which make up the different cuprates are widely used as a short-hand classification (*Crystal*

Structures of the High-T_c Superconducting Copper-oxides, H. Shaked *et al.* Elsevier Science, 1994, published as a special edition of *Physica C*).

The various cuprate superconductors are classified into subgroups according to their number of insulating and conducting CuO_2 planes per conducting block, and are presented in the ascending order of these planes. The naming scheme uses four numbers to represent the four possible types of layers that can potentially be present within the unit cell. The first number identifies the number of insulating layers between adjacent conducting blocks. These metal oxide layers typically contain the heavy metal atoms such as Hg, Tl, Pb or Bi. The second number represents the number of spacing layers that occur between identical CuO_2 blocks. There are always two of these spacing layers per conducting block. The infinite layer structure $(Ba,Sr)CuO_2$ represents a special case of the series 02′*n*–1′*n*, where *n* approaches infinity. These spacing oxide layers normally adopt the rock salt structure. The metal atoms normally found in the spacing layer include Ba, Sr and La. The third number gives the number of layers that separate adjacent CuO_2 planes within the conducting block. The metals typically found in the separating plane are Ca, Sr and rare earth elements. Finally, the fourth number is the number of CuO_2 planes within a conducting block. The four numbers are determined for one conducting block. For example, Tl Ba_2 Ca_2 Cu_3 $O_{9+\delta}$ can be represented as 1223, that is, containing (per conducting block) one insulating TlO layer, two spacing BaO layers, two separating elemental Ca layers, and three conducting CuO_2 planes (see Fig. 2).

This scheme of classification is not without its problems. The atomic positions of oxygen atoms can lead to a lack of uniqueness (*Crystal Structures of the High-T_c Superconducting Copper-oxides*, H. Shaked *et al.* Elsevier Science, 1994). For example, the materials $YBa_2Cu_3O_7$, $YBa_2Cu_4O_8$ and $Y_2Ba_4Cu_7O_{15}$ are commonly referred to by the three number names as 123, 124 and 247, respectively. These labels alternatively delineate the stoichiometry of the metal atoms without regard to their positions in the structure. With the four number system, 123 is a 1212 type; 124 is a 2212 type and 247 is an intergrowth of the 1212 and 2212 types.

The oxygen stoichiometry is of fundamental importance in determining the superconducting transition temperature, T_c. $YBa_2Cu_3O_{7-\delta}$ and the other 123 cuprates of the general formula Re $Ba_2Cu_3O_7$ (Re = rare earth element other than Ce, Pr, Tb) show superconductivity with a T_c of about 90 K in the near

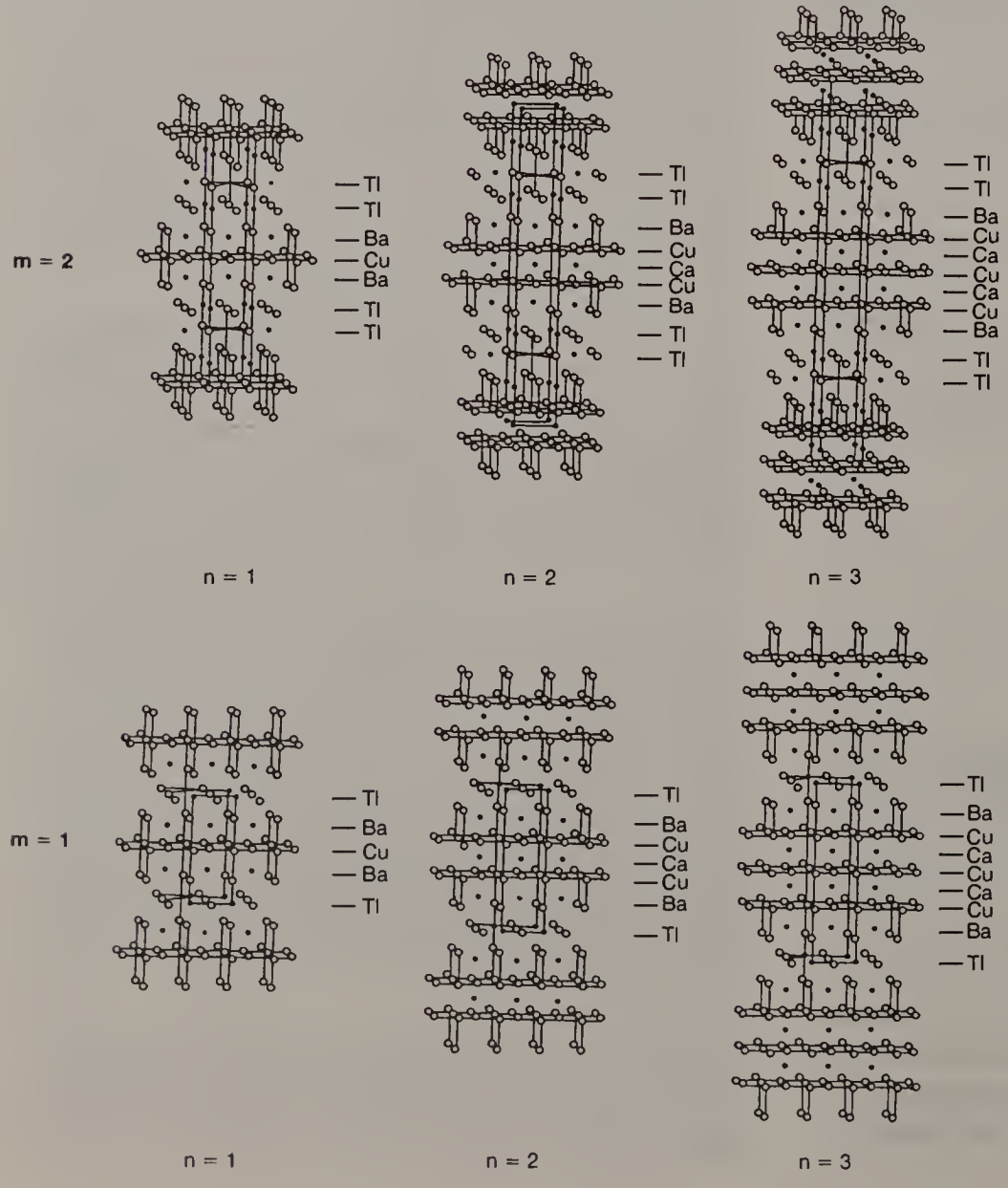

Fig. 2 Schematic representations of the structures of Tl cuprate superconductors of the type $Tl_mCa_{n-1}Ba_2Cu_nO_y$ for various *n*, when *m* = 1 or 2 (taken from C.N.R. Rao, *Chemistry of Advanced Materials*, Blackwell Scientific Publications, 1993).

stoichiometric compositions ($\delta \leq 0.2$). T_c is nearly constant up to $\delta = 0.2$ and then drops to about 60 K for $\delta = 0.3$–0.4 and finally reaches 45 K when $\delta = 0.5$.

$YBa_2Cu_3O_{6.5}$ ($\delta = 0.5$) is an oxygen vacancy-ordered structure with fully oxidized Cu–O chains alternating empty chains—as seen in Fig. 3. $YBa_2Cu_3O_{6.75}$ also seems to have a vacancy-ordered structure, but compositions with δ between 0.3 and 0.4 ($T_c \approx 60$ K) show no such ordering. It has been shown that this composition range is metastable, disproportionating to orthorhombic and tetragonal phases on annealing at low temperatures. Every oxygen atom added in this d range oxidizes Cu^+ in the chains without adding extra holes to the CuO_2 sheets, thereby giving rise to the variation of T_c.

The high temperature superconductors are all cuprates containing planes with copper ions in a square lattice. Under normal conditions, they all have a Cu^{2+} valence, and a strong Coulomb repulsive interaction suppresses charge fluctuations and gives rise to an insulating character. The parent compound of many of the cuprate superconductors, La_2CuO_4 (without any barium in the lattice), is not superconducting—it is antiferromagnetic. That is, the unpaired spins on the Cu^{2+} ions in the crystal are aligned parallel throughout the structure. The presence of this strong magnetic interaction locks the electrons to the lattice, stopping both conductivity and superconductivity. However, when some barium (Ba^{2+}) is introduced into the lattice replacing some lanthanum (La^{3+}) some compensation of charge has to be made to retain electrical neutrality. For every Ba^{2+} present, one Cu^{II} must be oxidized to Cu^{III}, or one O^{2-} reduced to O^-, and this effectively breaks up the alignment of the unpaired spins. When the average oxidation state of the copper ions reaches a critical value of about 2.2, the antiferromagnetism disappears and superconductivity appears.

Thus Superconductivity occurs only when the planes are doped to give a small number of Cu^{3+} ions. By contrast, conventional low temperature superconductors are metals with freely moving electrons. A number of theoretical proposals suggest that in the cuprate superconductors, the magnetic interactions of the spins of the Cu^{2+} ions cause *d*-wave electron pairs to form, minimizing Coulombic repulsion. Thus the successful experimental identification of *d*-wave properties in a superconducting cuprate would help to support these models and theories. However, the determination of the pair's internal state has proven difficult, because superconductivity is a consequence only of the coherent motion of the pairs, that is, the motion of all of the electron pairs, and is not sensitive to the relative motion of electrons in any one pair.

To investigate the internal state of the electron pair, early experiments measured the energy spectrum of

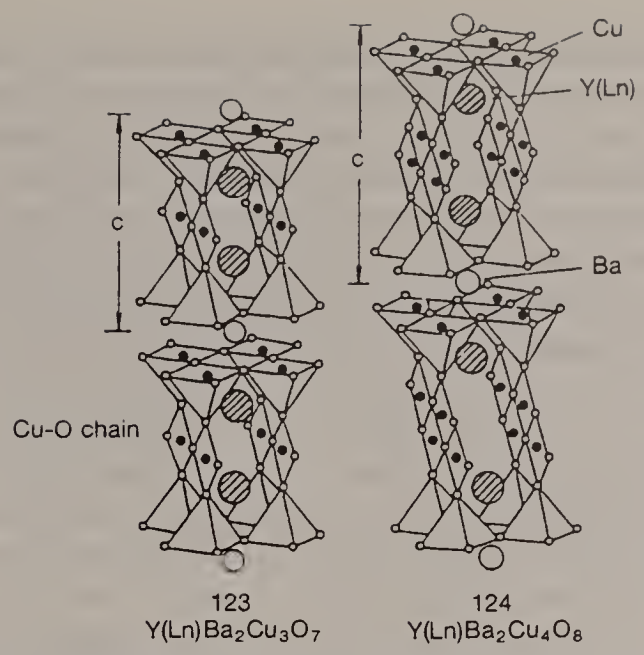

Fig. 3 Comparison of the structures of Y-123 and Y-124. In these structures there are Cu–O chains linking the CuO_2 layers, such chains do not exist between the CuO_2 layers present in the structures shown in Fig. 2 (taken from C.N.R. Rao, *Chemistry of Advanced Materials*, Blackwell Scientific Publications, 1993).

the excitations from the fully coherent ground state, that is, observed high-resolution emission spectra from high-quality single crystals of superconducting (low temperature) samples. The *s*-wave model suggests that any ejected photoelectron will be emitted from the sample isotropically—in all directions. If the emitting species has spherical symmetry, like an atomic *s*-orbital, then the probability of emission in any one direction would be the same as the probability of emission in any other direction. However, the pairing amplitude for *d*-wave pairs varies with direction, as with *d*-orbitals in atoms, with opposite sign along the *x* and *y* axes of the planes in the crystal. A plot of pairing amplitude as a function of angle would therefore look like a circle for *s*-wave states and a four-leaf 'clover' for *d*-wave states.

Such angle-resolved photoemission experiments at Stanford University, USA, which can resolve the angular dependence of the emitted photons, revealed small energy excitations along the $x = \pm y$ direction—as expected for *d*-wave superconductors. Similarly, recent low temperature measurements on high-quality samples by a group at the University of British Columbia, Canada, showed that the penetration depth within the superconductor (that is, the depth to which an applied magnetic field may penetrate a superconducting material), did not depend exponentially on the temperature, as is the case demanded by many theories of *s*-wave superconductors.

The key feature of *d*-wave pairing lies in the sign change of the pairing amplitude with angle. A breakthrough in the characterization of the electronic pairing state of high temperature superconductors occurred when experiments were devised which probed the spatial behaviour of the pairing amplitude. A recent test has

been the fabrication of superconducting circuits with built-in frustration. Groups at the University of Illinois, USA and ETH, Zurich, made interference devices (SQUIDs—Superconducting Quantum Interference Devices) which work on the Josephson effect, that is, that when two superconducting domains are separated by a very narrow nonsuperconducting layer there will be an measurable interference between the two superconducting layers—a quantum mechanical tunnelling across the intervening layer which is manifest as a small current flowing across the barrier. These SQUIDs were connected to the *x* and *y* axes of a high temperature superconducting sample to a conventional *s*-wave superconductor. Measuring the response of the SQUID to an applied magnetic field showed clear evidence that the pair amplitude had a sign change at one of the two superconducting junctions. That is, the measured interference pattern arising from the quantum mechanical tunnelling at a Josephson junction comprising an *s*-type superconductor and the *x* and *y* axes of a high temperature superconductor were different. This sign change is directly measurable by transferring Cooper pairs from a conventional *s*-type superconductor into the cuprate superconductors (perhaps *d*-type) at a variety of angles.

However, not all experiments support the *d*-wave hypothesis, and efforts are currently underway to establish if the remaining contradictions are apparent or real. However, these new types of experiments clearly tip the balance in favour of *d*-wave symmetry. Such experiments are fundamental to our understanding of the microscopic structure of this spectacular phenomenon. The fact that simple pictures of atomic orbitals, familiar to most chemists, can be applied to such exotic solid state phenomena as high temperature superconductivity clearly shows the interdependence of the fields of physical science.

However, what of practical applications? Even though we are still unsure of the mechanism of high temperature superconductivity, can we use it? After all, we know they work. Probably the first necessary, indeed, essential application will be wires made from these cuprate superconductors. Except for a few niche applications, for example, electromagnets for NMR medical imaging, the cost and inconvenience of using helium refrigeration has limited the widespread use of superconductors. With the cuprate superconductors, one should in principle be able to use, vastly cheaper, liquid nitrogen as a refrigerant. But what of the means of carrying the current at liquid nitrogen temperatures?

At the Spring Meeting of the Materials Research Society, San Francisco, USA, April 1995, a group from the Los Alamos National Laboratory (S. R. Foltyn *et al.*), USA, announced a world-breaking record current carrying capacity at 77 K. The result was obtained with thick films of $YBa_2Cu_3O_{7-\delta}$ (Y-123 or 1212 in the above classification), which has a transition temperature T_c = 92 K, deposited on flexible metal tapes 5 cm long by 1 cm wide. These tapes, which were only a few tenths of a millimetre thick, were coated by powerful pulsed laser deposition with Y-123 films of 1–2 mm. The Y-123 films were capable of carrying more than 100 A, with a critical current capacity of over 10^6 A/cm^2, well above the requirements for electrical transmission lines. The tapes were even capable of this current carrying behaviour while coiled and bent.

Y-123 has been the material of choice for such applications at liquid nitrogen temperatures because it retains high critical currents in epitaxial films or single crystals. This property is a direct consequence of the stronger vertical coupling between copper oxygen planes provided by the CuO chains in its crystal structure (see Fig. 3). Such cross-linking between the CuO_2 layers gives added mechanical stability when making deformed thin films.

Letters/Comments to the Editor

In the May, 1996, issue of *Chemistry International* (*CI,* Vol. 18, page 97) we published an figure taken from the set of teaching aids, DIDAC-1, produced by AGFA-GEVAERT for chemistry teachers. The image in question purported to show the toxicity of the various chemical elements. The following letter has been received concerning this figure.

Sir: As a toxicologist and a member of the IUPAC Commission on Toxicology, I was concerned to see the above figure being published with the implied blessing of IUPAC. It is profoundly misleading to classify elements as toxic or nontoxic. If I point out that the majority of compounds classified for human protection as having varying degrees of toxicity are carbon compounds and yet the AGFA-GEVAERT figure shows carbon as having no toxicity, you will see what I mean. Similarly, I see magnesium classified as harmful and yet I know that I need a millimolar solution in each cell of my body in order to stay alive. Fluorine is classified in the figure as very toxic and yet millions of people take fluoride in

their drinking water or in toothpaste for the good of their teeth. The truth is that elements as such should not be classified as toxic but only the forms in which they exist, that is—the chemical species. Thus, chlorine gas is highly toxic but chloride ions are essential for life.

Of course, the fundamental rule of toxicology is that any substance is toxic in a high enough dose. Thus, every substance may be classified as toxic but this does not contribute much to the safe use of chemical which is our prime concern.

The Commission on Toxicology is very concerned that classification of elements on a generic basis should cease and be replaced by proper consideration of chemical species. The AGFA-GEVAERT figure is not helpful in this respect.

I hope that AGFA-GEVAERT will revise their teaching aids to take my comments into account as I am sure that such aids can be a very valuable contribution to chemistry teaching and it would be unfortunate if they were spoiled by a naive and misleading classification of toxicity.

Yours sincerely,

Dr John Duffus
Heriot-Watt University, Scotland (UK)

Prague Meetings on Macromolecules

Dr Pavel Čefelín,

Due to unsatisfactory editing of the original text of this article it is here being reprinted.

Prague Meetings on Macromolecules (P.M.M.) are well known to many of those who are engaged in the research of macromolecular compound and their systems. Since monothematic microsymposia and discussion conferences in the series of P.M.M. have been mostly held under the auspices of IUPAC and therefore passed for the IUPAC monothematic meetings on macromolecules, it might be of interest to mention here the past of the P.M.M. and to inform of their future programme.

It was after the IUPAC International Symposium on Macromolecules in Prague in 1965 (MACRO 65), when Dr Blahoslav Sedláček, the then Scientific Secretary of the Institute of Macromolecular Chemistry of the Czechoslovak Academy of Sciences in Prague, started to implement his vision of the annual P.M.M. as monothematic microsymposia and discussion conferences on macromolecules which were to be sponsored by the just constituting IUPAC Macromolecular Division. A meeting was envisaged to consist of plenary sessions only, at which invited main lectures, special communications, and discussion contributions would be presented; more discussion sessions were to be scheduled at discussion conferences. The first P.M.M. microsymposium took place in 1967, and the P.M.M. soon gained reputation as meetings with highly specialized topics, careful preparation of scientific and social programmes, and versatile care of the participants. The original conception of P.M.M. has been maintained up to the present time. Dr Sedláček, the mastermind of P.M.M., chaired the P.M.M. Organizing Committee till 1972 and acted as the P.M.M. Editor afterwards (1973–1989).

Since 1967, thirty-six P.M.M. microsymposia (MS) and sixteen P.M.M. discussion conferences (DC) have been organized by the Institute of Macromolecular Chemistry in Prague: 1967—1st MS 'Polymer Gels and Concentrated Solutions'; 1968—2nd MS 'Structure of Organic Solids', 3rd MS ' Distribution Analysis and Fractionation of Polymers'; 1969—4th MS 'Rheology of Polymer Solids and Concentrated Solutions', 5th MS 'Cyclopolymers and Cyclopolymerization', 6th MS

Prague

'Light Scattering in Polymer Science'; 1970—7th MS 'Poly(vinyl chloride): Its Formation and Properties', 1st DC 'Models of Biopolymers: Structures and Functions'; 1971—8th MS 'Morphology of Polymers', 9th MS 'Thermodynamics of Interactions in Polymer Solutions'; 1972—2nd DC 'Macromolecular Matrices and Carriers of Biological Functions', 10th MS 'Conformational Structure of Polymers', 11th MS 'Mechanisms of Inhibition Processes in Polymers: Oxidative and Photochemical Degradation', 3rd DC 'General Principles of Rheology'; 1973—12th MS 'Organized Structures in Polymer Solutions and Gels', 13th MS 'Transformation of Functional Groups in Polymers'; 1974—14th MS 'Crosslinking and Networks', 4th DC 'Hetrogeneities in Polymers'; 1975—15th MS 'Degradation and Stabilization of Polymers'; 1976—5th DC 'Phases and Interfaces in Macromolecular Systems', 16th MS 'Advances in Scattering Methods'; 1977—17th MS 'Medical Polymers: Chemical Problems'; 1978—18th MS 'Synthetic and Semisynthetic Polymer Catalysts and Affinants', 6th DC 'Chromatography of Polymers and Polymers in Chromatography'; 1979—l9th MS 'Mechanisms of Degradation and Stabilization of Hydrocarbon Polymers', 20th MS 'Microcalorimetry of Macromolecules'; 1980—7th DC 'Polymer Networks', 21st MS 'Ring-Opening Polymerization of Heterocycles'; 1981—22nd MS 'Characterization of Structure and Dynamics of Macromolecular Systems by NMR Methods'; 1982—23rd MS 'Selective Polymeric Sorbents'; 1983—24th MS 'Copolymers: Structure and Solution Properties', 25th MS 'Long-Term Stabilities of Hydrocarbon Polymers'; 1984—26th MS 'Polymers in Medicine and Biology', 27th MS 'Physical Optics of Dynamic Phenomena and Processes in Macromolecular Systems'; 1985—28th MS 'Polymer Composites', 8th DC 'Morphology of Polymers'; 1986—29th MS 'Synthetic Polymer Membranes', 9th DC 'Crosslinked Epoxies'; 1987—30th MS 'Polymer-Supported Organic Reagents and Catalysts', 10th DC 'Small-Angle Scattering and Related Methods'; 1988—11th DC 'Chemical and Physical Phenomena in Ageing of Polymers', 31st MS 'Poly(vinyl chloride)'; 1989—12th DC 'Magnetic Resonance in Polymers', 32nd MS 'Polymer Blends'; 1990—13th DC 'Mechanisms of Polymer Strength and Toughness'; 1991—14th DC 'Rheology of Polymer Melts'; 1993—33rd MS 'Optics and Dynamics of Polymers', 34th MS 'Fluorinated Monomers and Polymers', 15th DC 'Wichterle's Days of Contact Lenses'; 1994—35th MS 'Polymer Netwoks'; 1995—36th MS 'High-Swelling Gels', 16th DC 'Morphology of Polymers', and 37th MS '(Bio)Degradable Polymers: Chemical, Biological and Environmental Aspects'. Periodicity in some evergreen topics is obvious. Since 1967 onwards, the series of P.M.M. was interrupted only once, in 1992, when the 34th IUPAC International Symposium on Macromolecules took place in Prague.

The following P.M.M., microsymposia and discussion conferences, are to be held with sponsorship of the IUPAC Macromolecular Division: 38th MS 'Recycling of Polymers' (14–17 July 1997), 17th DC 'Surface and Interfacial Phenomena in Macromolecular Systems' (21–24 July 1997), 18th DC 'Mechanical Behaviour of Polymeric Materials' (20–23 July 1998), 39th MS 'Advances in Polymerization Methods: Controlled Synthesis of Functional Polymers' (12–15 July 1999), l9th DC 'Rheology of Polymer Systems' (19–22 July 1999), 40th MS 'Polymers in Medicine' (17–22 July 2000), 20th DC 'Scattering Methods for the Investigation of Polymers' (9–12 July 2001), and 41st MS 'Polymer Membranes' 16–19 July 2001).

The author, Dr Pavel Čefelín, is the P.M.M. Coordinator and an Associate Member of the Macromolecular Division Committee of IUPAC. (Address: P.M.M. Secretariat, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám. 2, 162 06 Praha 6, Czech Republic.).

News

Secretariat News

Mr P.D. Gujral resigned from his position as Scientific Publications Secretary, effective 2 August 1996. Until further notice, all relevant documents and correspondence should be addressed to Miss M. K. Welch, Assistant Secretary Scientific Publications.

Dr Jeffrey H. Williams has resigned from his position as Deputy Executive Secretary of IUPAC and Editor of *Chemistry International,* effective 15 December 1996, to become the Secretary General of the European Physical Society. Until further notice, all relevant documents and correspondence should be addressed to Mrs Mary E. Patterson, Assistant Secretary Information Officer.

Names and addresses

Full details (names, addresses, telephone/telex/Fax numbers and E-mail) of the officers of IUPAC bodies were published in *Chemistry International* 1995, **17**(6),

215–226. The IUPAC Secretariat have been notified of the following changes:

Prof. John. E. Bertie (Chairman, Commission I.5), E-mail: john.bertie@ualberta.ca

Dr A. Cornish-Bowden (Chairman, IUBMB–IUPAC Joint Commission on Biochemical Nomenclature), E-mail: athel@ibsm.cnrs-mrs.fr

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Dr John T. Herron (Chairman, Commission I.4), Room A111, Physics Building, National Institute of Standards and Technology, Gaithersburg, MD 20899, USA.

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Prof. Gianfranco Scorrano (President, Organic Chemistry Division), E-mail: scorrano@pd.chor.chor.unipd.it

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Dr Yecheskel Wolman (Chairman, *Pure and Applied Chemistry* Editorial Advisory Board), Department of Organic Chemistry, Hebrew University of Jerusalem, Jerusalem 91904, Israel; Tel: +972 (2) 584501; Fax: +972 (2) 66804, 660346; E-mail: cheskea@vms.huji.ac.il

IUPAC colleagues deceased

UK: Dr. L. A. K. Staveley (8 February 1996), Physical Chemistry Division Committee (1963–1967), Commission on Physicochemical Measurements and Standards (1957–1975).

UK: Prof. H. A. Skinner (14 May 1996)—Physical Chemistry Division Committee (1965–1969), Commission on Thermodynamics (1957–1969).

Brazil: Prof. E. Giesbrecht (20 July 1996)—Committee on Teaching of Chemistry (1971–1977, 1979–1989), Commission on Atomic Weights and Isotopic Abundances (1991–1993).

Sweden: Prof. A. Magnéli (22 July 1996)—Inorganic, Chemistry Division Committee (1971–1975), Commission on High Temperature and Solid State, Chemistry (1969–1985).

Germany: Prof. J. H. Block (23 July 1995)—Commission on Colloid and Surface Chemistry including Catalysis (1979–1991).

Switzerland: Dr R. Morf (5 August 1996)—Secretary General of IUPAC (1955–1971), Finance Committee (1970–1972).

Dr R. Morf

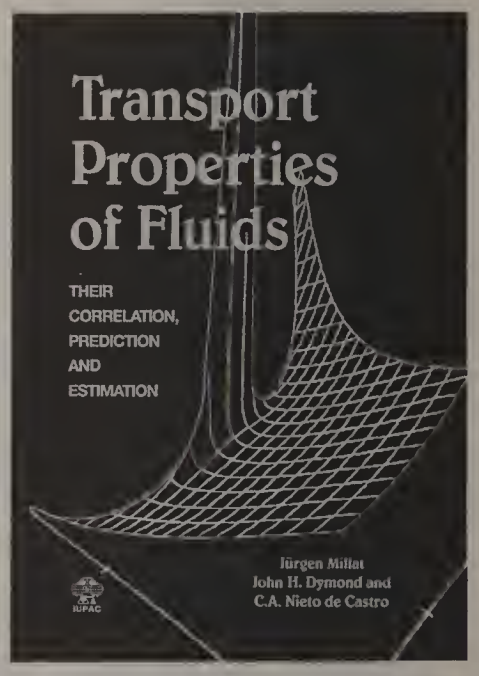
New publications

Transport properties of fluids: their correlation, prediction and estimation

The Commission on Thermodynamics of the Physical Chemistry Division of the International Union of Pure and Applied Chemistry is charged by the Union with the duty to define and maintain standards in the general field of thermodynamics. This duty encompasses matters such as the establishment and monitoring of international pressure and temperature scales, recommendations for calorimetric procedures, the selection and evaluation of reference standards for thermodynamic measurements of all types and the standardization of nomenclature and symbols in chemical thermodynamics. One particular aspect of the commission's work from among this set is carried forward by two subcommittees: one on thermodynamic data and the other on transport properties. These two subcommittees are responsible for the critical evaluation of experimental data for the properties of fluids that lie in their respective areas and for the subsequent preparation and dissemination of internationally approved thermodynamic tables of the fluid state and representations of transport properties.

The Subcommittee on Transport Properties has discharged its responsibilities through the work of groups of research workers active in the field drawn from all over the world. These groups have collaborated in the preparation of representations of the viscosity, thermal conductivity and diffusion coefficients of pure fluids and their mixtures over wide ranges of thermodynamic states. The representations have almost always been based upon an extensive body of experimental data for the property in question accumulated over many years by the efforts of laboratories world-wide. The results of this work have been published under the auspices of the subcommittee, with international endorsement, in *Journal of Physical and Chemical Reference Data* and *International Journal of Thermophysics*. The series of papers produced provides equations that describe the properties as a function of temperature and density that can be readily coded to yield transport properties at any prescribed thermodynamic state with a defined uncertainty.

In 1991, in collaboration with the Commission on Thermodynamics, the Subcommittee on Transport Properties brought together a wider group of experts to contribute to Volume III in the series *Experimental Thermodynamics,* which was edited by W. A. Wakeham, J. V. Sengers and A. Nagashima under the title *Measurement of the Transport Properties of Fluids* (Blackwell Scientific Publications, Oxford). The volume describes the state of the art with respect to the instrumentation for the determination of the transport properties of fluids which has been employed in the acquisition of the data upon which many of the representations of the properties have been based. However, the representations of the transport properties of fluids have also relied heavily on the use of kinetic theory to fill gaps for thermodynamic states where no experimental results exist or for properties where measurements have not been performed. The theory is then employed as a secure means of interpolation or even extrapolation from a smaller set of high-quality information.



The present volume was conceived by the Subcommittee on Transport Properties and the Commission on Thermodynamics to be a complement to the description of experimental techniques. Its purpose is therefore to outline the principles that underlie the statistical mechanical theories of transport processes in fluids and fluid mixtures in a way that leads to results that can be used in practice for their prediction or representation and to give practical examples of how this has been implemented. The brief to the editors of this book from the subcommittee has been admirably fulfilled by the team of authors that they have assembled. The coverage of the theory of transport properties is concise yet comprehensive and is developed in a fashion that leads to useful results. The sections on applications work their way through increasingly complicated archetypal systems from the simplest monatomic species to dense mixtures of polyatomic fluids of industrial significance and always with the emphasis on practical utility. This approach is concluded with examples of practical realizations of the representations of the properties incorporated in computer packages.

W. A. Wakeham (Chairman, Commission on Thermodynamics)

Introduction

Accurate knowledge of transport properties of pure gases and liquids, and of their mixtures, is essential for the optimum design of the different items of chemical process plants, for determination of intermolecular potential energy functions and for development of accurate theories of transport in dense fluids. A previous IUPAC volume, edited by Wakeham *et al.* (1991), also produced by Commission I.2 through its Subcommittee on Transport Properties, has described experimental methods for the accurate determination of transport properties. However, it is impossible to measure these properties for all industrially important fluids, and their mixtures, at all the thermodynamic states of interest. Measurements therefore need to be supplemented by theoretical calculations.

This present volume, which is complementary to the previous publication, discusses the present state of theory with regard to the dilute-gas state, the initial density dependence, the critical region and the very dense gas and liquid states for pure components and mixtures. In all cases, the intention is to present the theory in usable form and examples are given of its application to nonelectrolyte systems. This will be of particular use to chemical and mechanical engineers. The subtitle of this volume 'Their correlation, prediction and estimation' reflects the preferred order of application to obtain accurate values of transport properties. Careful correlation of accurate experimental data gives reliable values at interpolated temperatures and pressures (densities), and at different compositions when the measurements are for mixtures. Unfortunately, there are only a limited number of systems where data of such accuracy are available. In other cases, sound theoretical methods are necessary to predict the required values. Where information is lacking—for intermolecular forces, for example—estimation methods have to be used. These are of lower accuracy, but usually have more general applicability.

In view of the outstanding need for accurate theoretical prediction, this volume gives a clear presentation of current theory as applicable to fluids and fluid mixtures in different density ranges. As a result of the substantial advances made in recent years it is now possible to describe exactly the low-density transport properties as well as the critical enhancements.

The dilute-gas theory is presented here for the first time in terms of effective collision cross sections in a comprehensive readily usable form which applies to both polyatomic fluids and monatomic fluids. This description should now be used exclusively but, because it is relatively new, expressions are given for the macroscopic quantities in terms of these effective cross sections, and certain simple relationships between these effective cross sections and the previously used collision integrals are also described.

It is possible to account for the initial density dependence (at least for viscosity) and, although the description is not rigorous, it is sufficient for this often relatively small contribution to the transport properties. For higher densities, the modified Enskog theory can be used in a consistent manner, although this does have limitations. This becomes obvious from the fact that different empirical modifications have been proposed and applied to different regions of the transport property surface. Therefore, for certain ranges of thermodynamic states, an empirical estimation scheme based on the density dependence of the excess transport property is frequently to be preferred. For liquids and dense gases under conditions where the critical enhancements are negligible, methods based on hard-sphere theory give the best representation of experimental data.

Although experimental transport properties are measured at different temperatures and pressures, it is the density, or molar volume, which is the theoretically important variable. So, for the prediction of transport properties, it is necessary to convert data at a given temperature and pressure to the corresponding temperature and density, or vice versa, by use of a reliable equation of state. Accordingly, an account is given in this volume of the most useful equations of state to express these relationships for gases and liquids. For dense fluids, it is possible to calculate transport properties directly by molecular simulation techniques under specified conditions when the molecular interactions can be adequately represented. A description is included in this book of these methods, which are significant also for the results which have aided the development of transport theory.

When the above methods fail, estimation methods become important. Schemes based on the Corresponding-States Principle which are particularly important in this respect are described. In order to demonstrate clearly just when the methods of correlation, the theoretical expressions and estimation techniques are applicable, examples are given of transport-property data representation for systems of different complexity: simple monatomic fluids, diatomic fluids, polyatomic fluids (specifically, water and refrigerant R134a), nonreacting mixtures and (dilute) alkali-metal vapours as an example of a reacting mixture.

Rapid access to transport property data is essential for the efficient use of proposed correlation and prediction schemes. As a result, experimental data have been stored in many data banks world-wide and the final section of this volume describes a number of the major data banks, which also incorporate methods for the calculation of transport properties.

The authors are aware of the fact that, although this

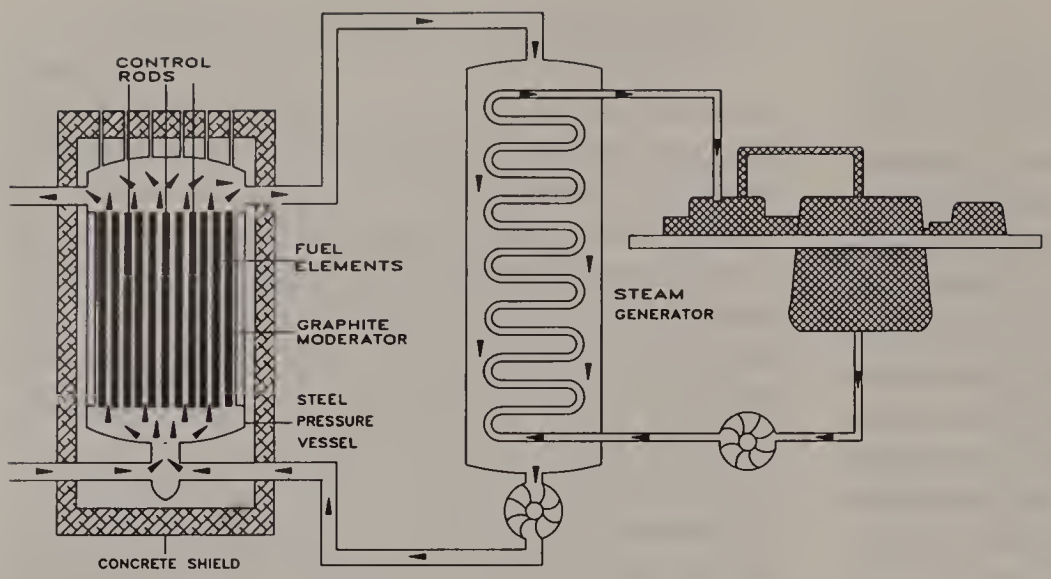


Fig. 1 A schematic diagram of a Magnox nuclear power plant

book demonstrates the significant progress that has been made in this field in the past decade, there is still a need for additional experimental and theoretical work in many parts of the transport-property surface. In the individual chapters, an attempt is made to specify the relevant needs in each density domain. It should be noted that this volume is restricted to a discussion of nonelectrolytes. In spite of their technological importance, ionic systems, including ionized gases and plasmas, molten metals and aqueous electrolyte solutions are not included because of the different nature of the interaction forces. A complete description of the transport properties of these fluids and fluid mixtures would occupy another volume.

The editors acknowledge with thanks the contributions which have been made by all the authors. They have attempted to produce a reasonable uniformity of style and apologize for any gross inconsistencies which remain. It is appreciated that not all theories of transport and estimation methods have been covered. For these omissions, and for all errors, the editors accept full responsibility. Finally, it is with the greatest pleasure that the editors acknowledge the support of members and corresponding members of the IUPAC Subcommittee on Transport Properties of Commission I.2 on Thermodynamics. Particular thanks are extended to its chairman, Professor W. A. Wakeham, for his many constructive comments and his unending enthusiasm and encouragement throughout.

J. Millat (NORDUM Institut für Umwelt und Analytik, Kessin/Rostock, Germany), J. H. Dymond (The University, Glasgow, UK) and C. A. Nieto de Castro (University of Lisbon, Portugal)

Many may think that a study of transport properties has only slight implications for everyday life, however, this book amply details many applications of the transport properties of fluids to many diverse engineering applications, for example, nuclear reactor safety.

Figure 1 contains a schematic diagram of a natural uranium graphite-moderated (Magnox) nuclear reactor. In a nuclear reactor the energy produced by the self-sustaining fission of a material such as ^{235}U is used to generate heat, which is transferred to a coolant circulating through the reactor. In turn, the heat absorbed by the coolant stream is transferred to a steam generator, which is then used to power a turbine for electricity generation. In the Magnox reactor the coolant is carbon dioxide at a pressure of 2 MPa, which leaves the reactor core at a temperature of 670 K. The reactor core itself is typically 14 m in diameter and 8 m high and is contained in a steel or concrete pressure vessel. The safety of such reactors has, quite naturally, caused considerable public concern, and their design, as well as that of other nuclear installations, is the subject of national legislation and international regulation. In particular, the safety audit for such a reactor must consider the circumstances surrounding the failure of one or more components in the entire plant. Thus, in addition to design calculations for the heat-exchange processes, one must consider extreme conditions when, for example, there is a loss of pressure in the coolant cycle or a failure of circulation for some reason. Generally, these latter calculations form a part of the safety case for the installation, and quality assurance then dictates that every single numerical value for a physical property is validated and of an appropriate pedigree. Included in such validated data would be the transport properties of the coolant stream allowing for possible contaminants as a result of a variety of modes of failure. The implication of the need for validated data implies high accuracy and a degree of approval from an appropriate body. In many cases, data produced by a body such as IUPAC (Vesovic *et al. J. Phys. Chem. Ref. Data* 1990, **19**, 763–808), which have international approval, would be deemed satisfactory. It seems likely that owing to the internationalization in the trade of plant designs of all kinds, such international approval will become increasingly important in satisfying the demands of national regulatory bodies for quality assurance.

The book is intended to be useful for scientists and

engineers who have to make use of representations of transport properties in order that they should understand the methodology that lies behind published correlations as well as the limitations of the development. It is also intended to be a summary of the status of the field at a particular moment for practitioners of the subject. It is thus a book which is intended to bring the latest state of knowledge to bear on problems of practical importance through international collaboration and thus fulfil one of the main objectives of IUPAC.

***Transport properties of Fluids: Their Correlation, Prediction and Estimation**, Edited by J. Millat (NORDUM Institut für Umwelt und Analytik, Kessin/ Rostock, Germany), J. H. Dymond (The University, Glasgow, UK) and C. A. Nieto de Castro (University of Lisbon, Portugal). Published by Cambridge University Press, 1996; ISBN 0-521-46178-2 hardback; xiv and 483 pp.; GBP 60.*

Molten Salts Bulletin '*Sels Fondus*'

The latest bulletin, 1996 No.60, in this series has been produced and contains a recent bibliography and details of recent conferences and publications devoted to the study of molten salts. To continue this series of publications, interested readers are requested to send information and reprints concerning their work in this field to:

***Molten Salts Bulletin 'Sels Fondus'**, M. Gaune-Escard, Institut Universitaire des Systèmes Thermiques Industriels, UA 1168, Université de Provence, Centre St. Jérôme, 13397 Marseille Cedex 20, France.*

This journal may also now be found on the Internet at: *http://iusti.univ-mrs.fr/IUSTI_EDITION/bulletin.html*

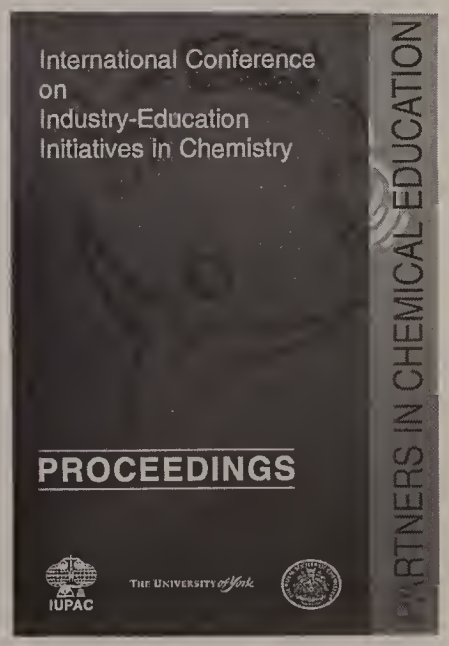
Partners in Chemical Education

The International Union of Pure and Applied Chemistry holds an International Conference on Chemical Education every two years. These have wide ranging topics such as: *Bringing Chemistry to Life* or *Teaching Chemistry in a Diverse World* or *Widening the Scope of Chemistry*. They are highly successful, attracting 500–700 chemical educators. However, there is also a place for meetings which have a much narrower objective and our group at the University of York (UK) suggested that IUPAC may wish to arrange these in years between the large meetings.

We suggested that the first topic should be concerned with the relationship between chemical education and industry. IUPAC's Committee on Teaching of Chemistry welcomed this proposal and asked us to arrange it and, happily, the Royal Society of Chemistry agreed to co-sponsor the event.

York, although delighted to arrange the meeting, realised that it had a tremendous responsibility to make it a success. York does have at least two advantages. First, it is a glorious city, surely one of the great European centres, dominated by the cathedral, York Minster, and many lovely buildings which illustrate its history from the days of its occupation by the Romans, 2000 years ago, through to today. Another advantage is the campus of the University (now about 30 years old) which is about 2 miles from the centre of the city and is built around a large lake. The facilities enable conference participants to work and be accommodated in very close proximity. Others, we hope, will think that York has other attributes, its Science Education Group and the Chemical Industry Education Centre, whose members did much of the hard work behind the scenes.

We chose the theme *Partners in Chemical Education* because of the growing enthusiasm for partnership between education and industry in many countries. We felt it was the right time to bring practitioners together, from both education and industry, to see and to discuss examples of work that had been produced from many parts of the world, to see examples of good practice and to see ways in which the partnerships can be initiated, developed and strengthened.



In an introduction to participants in the second circular we said that we wanted them to focus on:

Education about Industry. Learning about what industry does and how it does it helping to up-date teachers about teaching resources concerned with industry.

Education through Industry. *Using industrial practice, stories and activities to bring alive chemistry (or science) curricula.*

Education for Industry. Exploring teaching strategies which can help students develop skills needed in industry.

Education within Industry. Examination of the education and training provided within industry for its employees

For a partnership to succeed, all the partners must both contribute and get something in return which they value. Industry must know about, and understand, the changes in, and priorities, current educational practice, and, if they want any influence, to know what is needed from them. One of the important themes to come through was that Industry is interested in school education for two main reasons. One is to help ensure that it gets its fair share of talented and interested students. Another, increasingly, is to help in general education particularly in what is often referred to as public understanding of science. This is to ensure that the next generations are able to participate as effectively as possible in the debates that will surely emerge in societies that are increasingly dominated by advances in science and technology and huge changes in industrial practice.

In return, science education gains access to industry and industrialists which helps to keep its courses relevant, interesting and exciting and provide resources that can be used to do this. Increased knowledge of industry, its contribution to the economy, its inter-relationship with the environment are also valid and important elements of a modern science curriculum.

Thus, our overriding aim was to get the participants doing just that—to participate fully in the Conference. And further, we wanted to allow them to have as rich a menu as possible, to allow a wide choice. The reasons are simple. Too often, conferences are one way—a set of lectures and talks and too little real meeting of the minds and sharing of experiences. How often one hears the same comment—'the conference itself was OK but I got most benefit in the discussions over meals and in the bar afterwards!' A wide choice was needed to ensure that everyone went away feeling that the Conference gave something to them, while at the same time, they were able to give something to the Conference. This is not easy for we wanted educators from every sphere, from primary to tertiary, participants from industry and commerce to meet. We also wished to draw participants from as wide a spectrum of countries as possible.

So we designed a conference in which there was:

- only one major **plenary lecture** each day
- two groups of **invited lectures on chemistry** each day and given in parallel which illustrated themes of the meeting.

Then the centrepieces were:

- 20 **symposia,** the topics chosen being of interest to participants from the primary, secondary and tertiary sectors and from industry. In the first half of each symposium invited speakers gave short presentations followed by a brief question and answer session. The second half was devoted to the discussion of issues arising out of the questions being addressed. They were planned very carefully over the previous 18 months, with a great deal of correspondence between the symposia organizers and the other speakers.
- 20 **workshops** to provide participants with opportunities to work along side teams in leading areas of curriculum development and research in chemical education and so gain direct experience of new ideas for the teaching of chemistry at all levels. The participants were given the opportunity to gain 'hands-on' experience of each project, looking at printed materials, undertaking some of the activities suggested by the project as well as considering how they could transfer the philosophy, approach and/or materials into their own teaching. These were conducted by both chemical educators and industrialists.
- 70 **poster papers** were displayed which became the focal point of many informal discussions
- **Displays** were exhibited throughout the conference. These demonstrated how companies and organizations support the teaching of chemistry to 5 year olds, and up to, and including, undergraduates.
- A Conference newspaper, *Partners*, edited so nobly by Peter Childs and John Raffan, with help from Krishna Sane's group who were at the Conference in force, published daily. It made a fine start to each day, being distributed at breakfast.
- **Industrial visits** were arranged to four chemical sites and to CATALYST, the museum for the chemical industry. Each of these visits gave the participants time to see the site but also encouraged them to think about planning visits so that students would gain the maximum benefit from seeing an industrial plant first-hand.
- **Informal events** in the evening included a concert given by Concert Royal and a lecture on Mediaeval Glass in York Minster by Peter Gibson, Superintendent of the York Glaziers Trust. He is a marvellous lecturer on his equally marvellous work in which the restoration of the Rose Window damaged in the major fire in July 1984, is the centre piece.
- **Receptions** included one in Heslington Hall, given by the University. Heslington Hall is a mansion house which is over 400 years old, which is built in glorious red brick. The reception started there on the first evening and spread on to the lawns outside later on.
- **Visits** were arranged to the Minster and the Jorvik Centre, the new museum devoted to the recent excavations in York in which were found many new and exciting artefacts from the time the Vikings lived here. Other visits outside York were arranged, such as to the great house, Castle Howard, to the city of Durham, another city dominated by a magnificent cathedral, and to the Yorkshire Dales.

The Proceedings have now been published and they follow the pattern of the conference with sections devoted to the lectures, symposia, workshops and poster papers. The accounts of the symposia and workshops were drafted by participants not directly involved in setting them up and were edited afterwards. These drafts were produced by individuals who kindly gave their time to do this during the conference itself.

Although the poster papers were published as a separate booklet, as is usual in a Conference, and given to the participants, they contain a wealth of information and ideas. Thus we decided to republish them in the Proceedings. More than this, we asked several participants to enlarge their poster papers either because they were of special interest during the Conference or they illustrated in a particularly vivid way one of the themes of the meeting. Many others deserved this treatment but alas there was not the space we could devote to it, but all papers are being published in this volume, even from those few who, at the last minute, were unable to come to the meeting.

The Proceedings provide a picture of established collaboration between industry and education in several countries and the emergence of partnerships in many others. There is also a noticeable consistency in views expressed. For example, many industrialists stress the importance of skills such as communication and problem solving and these are key elements in an education for today. Teachers, on the other hand, are stressing the need for industry to listen to them in order to make industry's contributions more worthwhile—in particular in producing materials that are directly of use to their teaching. And everyone is agreed, careful planning and cooperation is needed before doing anything, whether for visits to industry, for industrialists going into schools, for the production of curriculum materials—indeed a true partnership is essential.

The Conference did not stop here, though. Throughout, as reflected in these pages, there are excellent examples of partnerships. Indeed, this leads us on to one final memory. One industrialist, from overseas, told us that he could come for one day. He enjoyed that so much, and found it so worthwhile, he cancelled his other engagements, and stayed with us for three. Amongst the nice compliments paid to us, that was the one that pleased us as much as any.

John Lazonby and David Waddington

***Partners in Chemistry, Procedings of the International Conference on Industry-Education Initiatives in Chemistry**; Published by the Chemical Industry Education Centre, Department of Chemistry, University of York, Heslington, York, YO1 5DD, UK; xiv +277 pages; ISBN 185342 561 3.*

World Health Organization Publications

Laboratory Techniques in Rabies

This manual provides an authoritative guide to the full range of laboratory techniques needed to support rabies control activities—whether involving diagnosis, prevention in dogs and wildlife, or the production and testing of human and animal vaccines. Now in its fourth edition, the manual has been thoroughly revised in line with considerable recent progress, particularly in the areas of molecular biology and immunology. Thirty new chapters are included. Although recently developed—and vastly improved—techniques are emphasized, the manual also explains how to achieve reliable results using classical method.

The manual has 47 chapters presented in six parts. Chapters in the opening part outline procedures for safe laboratory practice, introduce the different techniques needed in rabies diagnosis and research, and summarize the latest knowledge about the characteristics and molecular biology of the virus. Against this background, the seven chapters in part two provide detailed instructions for conducting routine procedures in rabies diagnosis and research. These range from the use of microscopic examination and histopathological diagnosis, through the mouse inoculation test, to the fluorescent antibody test, enzyme-linked immunosorbent assays (ELISAs) and cell cultures. Special diagnostic and research techniques are covered in part three, which describes procedures involving the use of monoclonal antibodies, the polymerase chain reaction, and purification techniques.

The most extensive part, on methods of vaccine production, contains seventeen chapters describing techniques for the production of human and animal brain-tissue vaccines, embryonating egg vaccines, and cell-culture vaccines. Genetically engineered vaccines for veterinary use are also covered. Although the superiority of cell-culture vaccines and purified avian embryo vaccines has been clearly demonstrated in humans, chapters on vaccines produced in suckling mice and adult sheep are included to assist the many countries where these vaccines continue to be used because of cost constraints.

Vaccine quality control is addressed in part five, which describes classical and new tests for potency, including antigen quantification. Advice on the comparative simplicity and economy of different tests is also provided. The final part covers techniques for the production and control of equine anti-rabies serum and human immunoglobulin.

Further practical advice is provided in a series of appendices, which describe techniques for the collection and shipment of brain specimens for rabies diagnosis,

preparation of rabies conjugates, and methods for the calculation of virus titres.

***Laboratory Techniques in Rabies**, Fourth edition, edited by F.-X. Meslin, MM. Kaplan and H. Koprowski 1996, xvii + 476 pages Available in English; French in preparation ISBN 92 4154479 1, CHF 115.-/USD 103.50 In developing countries: CHF 80.50. Order no. 1150426 from Distribution & Sales, WHO, 1211 Geneva 27, Switzerland.*

The World Health Report 1996: Fighting disease, Fostering development

The World Health Report 1996 provides an expert assessment of the world health situation in all its complexity, giving particular attention to infectious diseases. Compiled by the World Health Organization, the report combines the latest health statistics with an analysis of the many factors that have shaped the current situation—and created an unprecedented crisis.

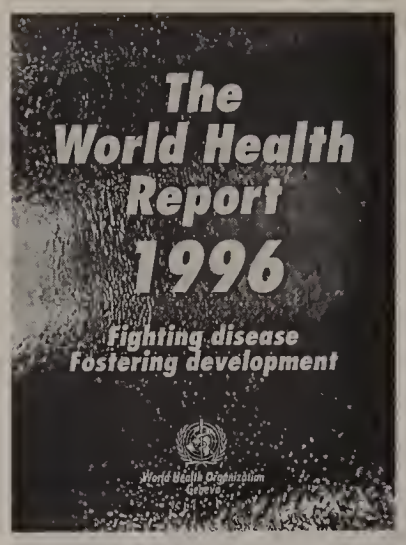
By showing where we stand today in the fight to control infectious diseases, the report aims to help the world comprehend both the alarming implications of recent trends and the need for immediate action. Over 50 old and new diseases from malaria, tuberculosis, and cholera to AIDS, plague and the mysterious Ebola haemorrhagic fever are profiled in terms of their incidence, causes, opportunities for control, and impact on health and socio-economic development.

The report opens with a profile of the state of world health at the end of 1995, including a concise analysis of global economic, political, social, and demographic trends relevant to health in general and infectious diseases in particular. Also included are the most up-to-date statistics on life expectancy, mortality by age group and sex, and causes of death and disease.

Against this background, the report turns to an in-depth analysis of infectious diseases. General problems considered include the emergence of several new diseases, the spread of epidemics, a sharp rise in antimicrobial resistance, and the growing number of hospital-acquired infections.

The most extensive section analyses over 50 diseases organized according to mode of transmission: person-to-person, contaminated food and water, insect bites, and contact with animals. By focusing on the way diseases spread, the report is able to trace how the present situation arose and identify the human interventions needed for prevention or control.

Throughout this analysis, the picture that emerges is one of a world poised to conquer some diseases soon, yet gravely threatened by many others, losing its arsenal of effective drugs, creating more and more opportunities for diseases to emerge or flourish, and above all paying a high price for past complacency.



As the report repeatedly argues, the price of continued complacency will be higher yet, especially since socio-economic development cannot move forward so long as so many of the world's people are disabled by disease.

To show the way forward, the report explains what WHO is doing to fight disease and foster development by combating these and many other problems. A final chapter, on charting the future, describes the precise actions needed to eradicate or eliminate diseases such as poliomyelitis, leprosy, neonatal tetanus, and guinea worm infection, to tackle old diseases such as tuberculosis and malaria, and to cope with several newer threats to health.

***The World Health Report 1996: Fighting disease, Fostering development 1996**, vi + 137 pages (available in English and French) ISBN 92 4156182 3; Order no. 1241996. CHF. 15.-/USD13.50; in developing countries: CHF 9. Copies may be obtained from Distribution & Sales, WHO, 1211 Geneva 27, Switzerland.*

The IUPAC Solubility Data

IUPAC Commission V.8 (Solubility Data) adopted, at its formation in 1979, the goal of preparing compilations of all experimental determinations of solubility reported in the world's chemical literature and, where possible, evaluating these data critically. This enormous task is approached by considering systems of two or more well defined components and producing printed volumes of compilations and critical evaluations of chemically related systems.

From 1979 to 1993 (to volume 53) these volumes of solubility data were published by Pergamon Press. Since 1994 (from volume 54) the volumes have been published by Oxford University Press. The two most recent volumes are:

Vol. 62. P. Scharlin, **Carbon Dioxide in Water and Aqueous Electrolyte Solutions** (1996)

Vol. 63. H.U. Borgstedt and C. Guminski, **Metals in Liquid Alkali Metals, Part I: Be to Os** (1996)

There will be a further two volumes published in 1996 by Oxford University Press, however, after this year the series will not continue to be published by Oxford University Press. A further announcement will be made as to the future publisher for the Solubility Data Series and to the future use of electronic means for the dissemination of these data compilations.

ISO Standards

The following are some of the new international standards announced by the International Organization for Standardization (ISO) in recent issues of *ISO Bulletin*.

New International standards published between 15 March 1996 and 13 April 1996

TC 102	**Iron ores**
ISO 11533:1996	Iron ores—Determinarion of cobalt content—Flame atomic absorption spectrometric method
TC 155	**Nickel and nickel alloys**
ISO 12169:1996	Nickel oxide—Determination of nickel contents—Electrolytic deposition method

New International Standards published between 13 May 1996 and 10 June 1996

TC 27	**Solid mineral fuels**
ISO 157:1996	Coal—Determination of forms of sulfur
TC 34	**Agricultural food products**
ISO 3961:1996	Animal and vegetable fats and oils—Determination of iodine value

New International Standards published between 11 June 1996 and 11 July 1996

TC 17	**Steel**
ISO 14284:1996	Steel and iron—Sampling and preparation of samples for the determination of chemical composition
TC 24	**Sieves, sieving and other sizing methods**
ISO 13321:1996	Particle size analysis—Photon correlation spectroscopy
TC 28	**Petroleum products and lubricants**
ISO 2049:1996	Petroleum products—Determination of colour (ASTM scale)
ISO 3648:1994/ Cor 1:1996	Technical Corrigendum 1
ISO 3837:1993/ Cor 2:1996	Technical Corrigendum 2
ISO 12185:1996	Crude petroleum and petroleum products—Determination of density—Oscillating U-tube method
ISO 13757:1996	Liquefied petroleum gases Determination of oily residues—High temperature method
TC 35	**Paints and varnishes**
ISO 7783–1: 1996	Paints and varnishes—Determination of water–vapour transmission rate—Part 1: Dish method for free films
TC 45	**Rubber and rubber products**
ISO 976:1996	Rubber and plastics—Polymer dispersions and rubber latices—Determination of pH
TC 85	**Nuclear energy**
ISO 9894:1996	Subsampling of uranium hexafluoride in the liquid phase
ISO 9989:1996	Determination of uranium in uranium dioxide powder and pellets—Iron(II) sulfate reduction/ potassium dichromate oxidation titrimetric method
TC 147	**Water quality**
ISO 7346–1: 1996acute	Water quality—Determination of the lethal toxicity of substances to a freshwater fish [Brachydanio rerio Hamilton–Buchanan (Teleostei, Cyprinidae)]—Part 1: Static method
ISO 7346–2: 1996acute	Water quality—Determination of the lethai toxicity of substances to a freshwater fish [Brachydanio rerio Hamilton–Buchanan (Teleostei, Cyprinidae)]—Part 2: Semi-static method
iSO 7346–3: 1996acute	Water quality—Determination of the lethal toxicity of substances to a freshwater fish [Brachydanio rerio Hamilton–Buchanan (Teleostei, Cyprinidae)]—Part S: Flow-through method
ISO 11969:1996	Water quality—Determination of arsenic—Atomic absorption spectrometric method (hydride technique)
ISO 13395:1996	Water quality—Determination of nitrite nitrogen and nitrate nitrogen and the sum of both by flow analysis (CFA and FIA) and spectrometric detection
TC 183	**Copper, lead and zinc ores and concentrates**
ISO 12745:1996	Copper, lead and zinc ores and concentrates—Precision and bias of mass measurement techniques
ISO 13543:1996	Copper, lead and zinc sulphide concentrates—Determination of mass of contained metal in a lot

Full details of these and ISO standards may be obtained from: ISO Central Secretariat, Case Postal 56, CH-1211 Geneva, Switzerland. Tel.: +41 22 749 01 11; Fax: +41 22 733 34 30.

Affiliate Affairs

Information for affiliates

IUPAC publications

Affiliates are entitled to a 25% reduction, and in some cases a 40% reduction on the cost of IUPAC publications except *Pure and Applied Chemistry.* A leaflet detailing IUPAC books currently available from Blackwell Science Ltd has recently been distributed by the publishers to all *CI* readers. Further copies may be obtained from the IUPAC Secretariat.

How to contact commissions

IUPAC affiliates may if they wish communicate directly on scientific matters with the officers of IUPAC commis-

sions. A full list of names and addresses of all commission officers for 1996–97 was published in the November 1995 issue of *CI*.

Affiliate reduction of conference registration fees

It is a condition of IUPAC sponsorship of a conference that IUPAC affiliates are entitled to a 10% reduction or 'own members' rate on the registration fee for scientific participants. This concession is usually, but not always, announced in the conference circulars and indicated on the registration form.

To receive this reduction an affiliate must declare on the conference registration form that (s)he is an affiliate. Alternatively the affiliate should apply in writing to the conference organizer for this reduction stating that (s)he is an affiliate. Conference organizers may check with the IUPAC Secretariat that applicants for this reduction are currently registered as affiliates.

If an application for this reduction is refused, an affiliate should immediately notify the Affiliate Affairs Secretary and, if possible, forward copies of documentary evidence of this refusal.

Ties and scarves

Ties and scarves emblazoned with the IUPAC logo may be purchased from the IUPAC Secretariat by applying to the Affiliate Affairs Secretary. The colours for both are *either* maroon *or* dark blue. The ties cost USD 14.00/GBP 7.00 each and the scarves USD 12.00/GBP 6.00 (including postage and packing).

Please use the form (or a photocopy of it) published on page 24 of the January 1994 issue of *CI*. Alternatively please write to the Affiliate Affairs Secretary with your order stating the colour you require. A cheque made payable to IUPAC for the appropriate amount should be enclosed with your order.

Visas

It is a condition of sponsorship that organizers of meetings under the auspices of IUPAC, in considering the locations of such meetings, should take all possible steps to ensure the freedom of all *bona fide* chemists from throughout the world to attend irrespective of race, religion, or political philosophy.

IUPAC sponsorship implies that entry visas will be granted to all bona fide chemists provided application is made not less than three months in advance. If a visa is not granted one month before the meeting the IUPAC Secretariat should be notified without delay by the applicant.

Address of IUPAC Secretariat

Please use the following address for all communications directed to the IUPAC Affiliate Affairs Secretary. If your are submitting a letter for publication in *Chemistry International* (*CI*), please indicate that the letter is 'Submitted for publication in *CI*.'

Affiliate Affairs Secretary, IUPAC Secretariat, Bank Court Chambers, 2–3 Pound Way, Templars Square, Cowley, Oxford OX4 3YF, UK.
Tel: +44 (0)1865 747744
Fax: +44 (0)1865 747510
E-mail: iupac@vax.oxford.ac.uk

IUPAC poster

Copies of an IUPAC poster are available **free of charge** to affiliates and members of IUPAC's commissions and committees. The poster is printed in maroon and black on a white background and is approximately 42 × 59 cm in size.

IUPAC welcomes any publicity you can give to its activities. If you would like to display one or more copies of the poster in your department or elsewhere please write to the Affiliate Affairs Secretary stating your name and address and how many copies of the poster you wish to receive.

IUPAC-sponsored conferences

An updated list of names and addresses of the organizers of all future IUPAC sponsored conferences is given in the 'Conference Calendar' published in each issue of *CI*.

Conference calendar

1997

Thermodynamics

5–8 January

International Symposium on Chemical and Biological Thermodynamics. Amritsar, India.
Prof. Bhajan Singh, Department of Chemistry, Guru Nanak Dev University, Amritsar-143005, India. Tel.: +91 (183) 258845. Fax: +91 (183) 258820. E-mail: bhajan@gndu.ernet.in

Recycling

4–7 February
International Recycling Congress (R'97). Geneva, Switzerland.
Dr A. Barrage, c/o LPM Limited, Tannenweg 10, CH-5712 Beinwil, Switzerland. Tel.: +41 (62) 7715555. Fax: +41 (62) 7715564. Further information about R'97 may be found on their Home Page: http://www.r97.ch/r97

Safety in chemical production

13–17 April
3rd IUPAC Workshop on Safety in Chemical Production: Environmentally sustainable Manufacture of Competitive Products. San Francisco, USA.
Dr A. M. Ford, Gulf Coast Hazardous Substance Research Centre, Lamar University, PO Box 10613, Beaumont, TX 77710-0613, USA. Tel.: +1 409 880 8768; Fax: +1 409 880 2397.

High temperature materials chemistry

19–23 May
9th International Conference on High Temperature Materials Chemistry (HTMC IX). Pennsylvania State University, PA, USA.
Prof. Karl E. Spear, Materials Science & Engineering Department, Pennsylvania State University, 118 Steidle Building, University Park, PA 16802, USA.

Bioorganic chemistry

1–6 June
4th International Symposium on Bioorganic Chemistry. Biarritz, France.
Prof. A. Marquet, Université Paris URA CNRS 493, Laboratoire de Chimie Organique Biologique, Tour 44/45-4 Pl. Jussieu, 75252 Paris Cedex 05, France.

Molecular architecture for degradable polymers

10–14 June
International Symposium on Molecular Architecture for Degradable Polymers: Molecular Design of Polymeric Materials of Tomorrow. Stockholm, Sweden.
Prof. Ann-Christine Albertsson, Department of Polymer Technology, KTH, Royal Institute of Technology, S-100 44 Stockholm, Sweden. Tel.: +46 (8) 7908274. Fax: +46 (8) 100775.

Polymer synthesis

16–20 June
International Symposium on New Approaches in Polymer Synthesis and Macromolecular Formation. St. Petersburg, Russia.
Mrs Irina Kovalenko (Symposium Coordinator), Institute of Macromolecular Compounds, Bolshoy pr. 31, 199004 St. Petersburg, Russia. Tel.: +7 (812) 2131070. Fax: +7 (812) 2186869. E-mail: imc@macro.spb.su

Ionic polymerization

7–11 July
International Symposium on Ionic Polymerization. Paris, France.
Prof. F. Cheradame, CNRS, BP 28, 2 rue Henri Dunant, 94320 Thiais, France.

Recycling of polymers

14–17 July
38th Microsymposium on Macromolecules, Recycling of Polymers. Prague, Czech Republic.
P.M.M. Secretariat, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám 2, 162 06 Prague c-Petriny, Czech Republic. Tel.: +42 (2) 360341. Fax: +42 (2) 367891. E-mail: sympo@imc.cas.cz

Interfacial phenomena

21–24 July
17th Discussion Conference on Macromolecules, Surface and Interfacial Phenomena in Macromolecular Systems. Prague, Czech Republic.
P.M.M. Secretariat, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám 2, 162 06 Prague c-Petriny, Czech Republic. Tel.: +42 (2) 360341. Fax: +42 (2) 367891. E-mail: sympo@imc.cas.cz

Bioinorganic chemistry

27 July–1 August
8th International Conference on Bioinorganic Chemistry. Yokohama, Japan.
Prof. M. Hidai, Department of Chemistry & Biotechnology, Graduate School of Engineering, The University of Tokyo, Hongo, Tokyo, Japan.

Plasma chemistry

18–22 August
13th International Symposium on Plasma Chemistry. Beijing, China.
Dr Lin He, The Chinese Society of Theoretical & Applied Mechanics, 15 Zhong Guan Cun Road, Beijing 100080, China.

IUPAC Congress

18–22 August
36th IUPAC Congress. Geneva, Switzerland.
36th IUPAC '97, c/o AKM Congress Service, PO Box 37, CH-1218 Le Grand-Saconnex/GE, Switzerland. Tel.: +41 (22) 7611661. Fax: +41 (22) 7611662.

IUPAC General Assembly

23–30 August
39th IUPAC General Assembly. Geneva, Switzerland.
The IUPAC General Assembly is not open for general participation but restricted to members of IUPAC bodies that meet on this occasion.

Coordination chemistry

24–29 August
32nd International Conference on Coordination Chemistry. Santiago, Chile.
Prof. J. Costamagna, Departamento de Química, Facultad de Ciencia, Universidad de Santiago di Chile, Casilla 307, Santiago-2, Chile. Tel.: +56 (2) 6811644. Fax: +56 (2) 6812108. E-mail: jcostama@lauca.usach.cl

Spectroscopicum internationale

21–26 September
30th Colloquium Spectroscopicum Internationale 1997 (CSI). Melbourne, Australia.
The Meeting Planners, 108 Church Street, Hawthorn Victoria 3122, Australia. Tel.: +61 (3) 98193700. Fax: +61 (3) 98195978.

Emulsions

23–26 September
2nd World Congress on Emulsion: Industrial Applications of Emulsions. Bordeaux, France.
Mr A. Le Coroller, Directeur-Général, CME, 50 place Marcel Pagnol, 92100 Boulogne-Billancourt, France. Tel.: +33 (1) 47617689. Fax: +33 (1) 47617465.

Biodiveristy and Bioresources

November
International Conference on Biodiversity and Bioresources—Preservation and Utilization. Phuket, Thailand.
Prof. Yongyuth Yuthavong, National Science & Technology Development Agency, Gypsum Metropolitan Tower, 18th Floor, 539/2 Sri-Ayudhya Road, Rajdhavee, Bangkok 10400, Thailand.

1998

Organic synthesis

30 June–4 July
12th International Conference on Organic Synthesiz. Venice, Italy.
Prof. C. Scolastico, Dip.to di Chimica Organica e Industriale, Università di Milano, Via G. Venezian 21, I-20133 Milano, Italy.

Macromolecules

20–23 July
18th Discussion Conference of Macromolecules: Mechanical Behaviour of Polymeric Materials. Prague, Czech Republic.
Dr Jaromir Lukás, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovského nám 2, 162 06 Prague 6 Petriny, Czech Republic.

Chemical thermodynamics

26 July–1 August
15th International Conference on Chemical Thermodynamics. Porto, Portugal.
Prof. M. A. V. Ribeiro da Silva, Department of Chemistry, Faculty of Science, Rua do Campo Alegre 687, P-4150 Porto, Portugal

Pesticide chemistry

2–7 August
9th International Congress on Pesticide Chemistry. London, UK.
Dr John F. Gibson, Secretary (Scientific), The Royal Society of Chemistry, Burlington House, London W1V OBN, UK. Tel.: +44 (171) 4378656. Fax: +44 (171) 7341227.

Physical organic chemistry

16–21 August
14th International Conference on Physical Organic Chemistry, Santa Catarina, Brazil.
Prof. E. Humeres, Universidade Federal de Santa Catarina, Departamento di Química, 88040-900 Florianópolis S.C. Brazil.

Coordination chemistry

30 August–4 September
33rd International Conference on Coordination Chemistry. Florence, Italy.
33rd ICCC Secretariat, Department of Chemistry, University of Florence, Via Gino Capponi 7, 50121 Firenze, Italy. Tel.: +39 (55) 2757549. Fax: +39 (55) 2757555.

Natural products

October
21st IUPAC Symposium on the Chemistry of Natural Products. Beijing, China.
Prof. Xiao-Tian Liang, Institute of Materia Medica, Chinese Academy of Medical Sciences, 1 Xian Nong Tan Street, Beijing 100050, China.

2000

Macromolecules

9–14 July
MACRO 2000: International Symposium on Macromolecules. Warsaw, Poland.
Prof. S. Penczek, Centrum Badan Molekularnych i Makromolekularnych, Polskiej Akademii Nauk, ul. Sienkiewicza 112, PL-90–363 Lodz, Poland. Tel.: +48 (42) 819815. Fax: +48 (42) 847126.

Biotechnology

3–8 September
11th International Biotechnology Symposium. Berlin, Germany.
Prof. G. Kreysa, DECHAEMA e.V., PO Box 15 01 04, D-60061 Frankfurt am Main, Germany.

Index

Affiliate Affairs 30, 72, 263
Affiliate Membership Programme 31
AMP in Cuba 73
Antimatter 97
Atomic Weights 50

Biophysical Chemistry Commission 214
Bohuslav Brauner 81
Brisbane '96 231

Chemical Abstracts Service 8
Chemical Education 259
Chemistry and the Environment 219
Chemistry Teaching on the WWW 239
Chlorine (White Book) 242
CODATA 222
Commission News 56, 209
Conference Calendar 38, 77, 117, 197, 229, 264
Conferences 35, 74, 116, 192, 226

Deceased Colleagues 29, 85, 173, 228, 255

Electronic Publishing 165

Femtosecond Chemistry 61

Groundwater Contamination 180

High T_c Superconductors 248

IOCD 41
ISO 203
ISO Standards 51, 183, 263
Istanbul IUPAC Congress 1
IUPAC Accounts 174
IUPAC Annual Report 169
IUPAC on the WWW 184
IUPAC–UNESCO Collaboration 86
IUPACSEARCH (4.1) 105, 190
IUPACSEARCH (4.2) 221

Joseph Bunnett 218

Korean Air Pollution 161

Letters to Editor 83, 252

Macromolecular Symposia 113, 186, 220
Macromolecules in Prague 163, 253
Metrology 91
Mixing 10

Names and Addresses 51, 99, 182, 255
New Publications 66
Nitric Oxide 214
Nobel Prizes for 1995 94
Nomenclature on the WWW 105

PAC Review 21, 52, 205
Phenothiazines 217
Provisional Recommendations 32, 183

Recent Reports 25, 99, 178, 225

SCOPE 222
Secretariat Changes 161
Secretary General 201
Silver Book 69
Solubility Data Series 47, 190, 262

Teaching of Chemistry 13
Thermodynamic Properties 256
Thieme–IUPAC Prize 213
Transport Properties 44

Water Structure 216

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Official Journal of the International Union of Pure and Applied Chemistry

EXECUTIVE EDITOR

P.D. Gujral, *IUPAC Secretariat, Bank Court Chambers, 2-3 Pound Way, Templars Square, Cowley, Oxford OX4 3YF, UK*

Since 1960 the Union has made available to chemists everywhere a very large amount of important material which it handles each year through its regular publication in Pure and Applied Chemistry. The objectives of the journal are:

- to publish the main invited lectures of symposia sponsored by IUPAC at which authoritative and up-to-date accounts of the subject of the symposium are presented by prominent scientists; the lecturers cover their own recent work and review the worldwide literature on the subject;
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- to publish critically evaluated state-of-the-art commissioned review articles on important topics.

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IUPAC Secretariat

Bank Court Chambers, 2–3 Pound Way, Templars Square, Cowley, Oxford OX4 3YF, UK.
Telephone: +44 (0)1865 747744. Fax: +44 (0)1865 747510. E-mail: iupac@vax.oxford.ac.uk

The International Union of Pure and Applied Chemistry (IUPAC), formed in 1919, is a voluntary non-governmental, non-profit association of organizations, each of which represents the chemists of a member country.

Its objectives are:

- to promote continuing co-operation among the chemists of the member countries;
- to study topics of international importance to pure and applied chemistry which need regulation, standardization, or codification;
- to co-operate with other international organizations which deal with topics of a chemical nature;
- to contribute to the advancement of pure and applied chemistry in all its aspects.

The membership of IUPAC presently comprises 40 countries, each represented by a national organization, such as an academy of science or research council.

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Australian Academy of Science **(Australia)**
Ôsterreichische Akademie der Wissenschaften **(Austria)**
Nationaal Comité voor Scheikunde/Comité National de Chimie **(Belgium)**
Brazilian Chemistry Committee for IUPAC **(Brazil)**
National Research Council of Canada **(Canada)**
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IUPAC

1996, Vol. 18, No. 6 (November)

231 Brisbane '96

239 Chemistry teaching and the Internet
Becky Allen

242 White Book on Chlorine

248 High temperature copper oxide superconductors

252 Letters/Comments to the Editor

253 Prague Meetings on Macromolecules
Dr Pavel Čefelín

254 News

256 New publications

263 ISO Standards

263 Affilate Affairs

264 Conference calendar

267 Index

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